Full wwPDB EM Validation Report

Sep 29, 2026 – 10:04 PM JST

PDB ID	:	9K7V / pdb_00009k7v
EMDB ID	:	EMD-62153
Title	:	Structural insights into photosystem II supercomplex of a a siphonous green algae Bryopsis corticulans from intertidal zone
Authors	:	Liu, X.Y.; Wang, W.D.
Deposited on	:	2024-10-24
Resolution	:	3.07 Å(reported)

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

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

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

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

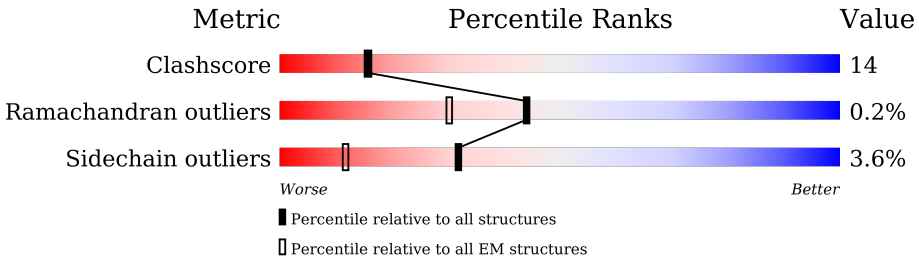
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

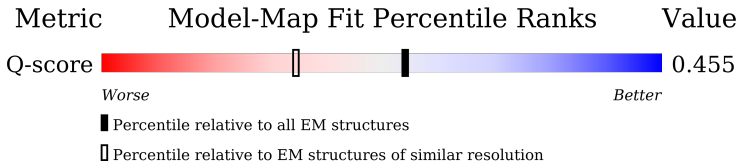
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.07 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	Z	62	77% 21%
1	z	62	84% 15%
2	E	82	51% 27% 21%
2	e	82	67% 12% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	75	64% 27% 9%
3	h	75	5% 63% 28% 9%
4	I	36	83% 11% 6%
4	i	36	83% 11% 6%
5	K	43	60% 23% 14%
5	k	43	72% 14% 14%
6	L	38	66% 26% 5%
6	l	38	63% 32%
7	M	33	9% 61% 30% 9%
7	m	33	9% 58% 30% 9%
8	R	267	16% 53% 29% 16%
8	r	267	17% 58% 24% 16%
9	F	42	55% 17% 26%
9	f	42	55% 17% 26%
10	1	212	58% 68% 30%
10	4	212	58% 73% 25%
11	2	256	10% 66% 20% 14%
11	5	256	9% 65% 21% 14%
12	3	254	54% 59% 23% 17%
12	6	254	58% 59% 26% 14%
12	7	254	56% 27% 14%
12	9	254	86% 53% 31% 14%
12	p	254	55% 27% 14%
12	u	254	86% 52% 32% 14%
13	S	308	51% 27% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	s	308	52% 26% 19%
14	X	109	28% 69%
14	x	109	28% 69%
15	V	33	42% 48% 21% 6% 24%
15	v	33	39% 52% 21% 24%
16	T	31	65% 26% 10%
16	t	31	65% 26% 10%
17	8	280	51% 22% 26%
17	G	280	60% 57% 22% 20%
17	N	280	45% 49% 22% 26%
17	Y	280	58% 22% 20%
17	g	280	60% 56% 24% 20%
17	n	280	45% 49% 23% 26%
17	q	280	51% 22% 26%
17	y	280	59% 21% 20%
18	B	508	70% 22% 6%
18	b	508	72% 21% 6%
19	A	327	70% 28%
19	a	327	72% 27%
20	C	461	5% 75% 21%
20	c	461	5% 74% 21%
21	D	352	74% 21%
21	d	352	74% 22%
22	W	118	29% 7% 64%
22	w	118	30% 7% 64%

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
28	NEX	1	303	-	-	X	-
28	NEX	3	318	-	-	X	-
28	NEX	4	303	-	-	X	-
28	NEX	6	303	-	-	X	-
28	NEX	7	304	-	-	X	-
28	NEX	G	304	-	-	X	-
28	NEX	S	617	-	-	X	-
28	NEX	p	304	-	-	X	-
28	NEX	s	401	-	-	X	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 95298 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 II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		
1	z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		

- Molecule 2 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	65	Total	C	N	O	0	0
			530	347	87	96		
2	e	65	Total	C	N	O	0	0
			530	347	87	96		

- Molecule 3 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	68	Total	C	N	O	S	0	0
			513	337	74	98	4		
3	h	68	Total	C	N	O	S	0	0
			513	337	74	98	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	34	Total	C	N	O	S	0	0
			275	189	40	45	1		
4	i	34	Total	C	N	O	S	0	0
			275	189	40	45	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	26	ASP	ASN	conflict	UNP A0A2P0QH95

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
i	26	ASP	ASN	conflict	UNP A0A2P0QH95

- Molecule 5 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	37	Total 299	C 208	N 43	O 48	0	0
5	k	37	Total 299	C 208	N 43	O 48	0	0

- Molecule 6 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	37	Total 304	C 204	N 48	O 52	0	0
6	l	37	Total 304	C 204	N 48	O 52	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	30	Total 231	C 159	N 33	O 39	0	0
7	m	30	Total 231	C 159	N 33	O 39	0	0

- Molecule 8 is a protein called PsbR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	225	Total 1711	C 1092	N 284	O 326	S 9	0	0
8	r	225	Total 1707	C 1089	N 283	O 326	S 9	0	0

- Molecule 9 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	31	Total 246	C 167	N 40	O 38	S 1	0	0
9	f	31	Total 251	C 170	N 42	O 38	S 1	0	0

- Molecule 10 is a protein called Lhcb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	212	Total	C	N	O	S	0	0
			1609	1038	255	306	10		
10	4	212	Total	C	N	O	S	0	0
			1603	1035	252	306	10		

- Molecule 11 is a protein called Lhcb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	221	Total	C	N	O	S	0	0
			1710	1108	278	316	8		
11	5	221	Total	C	N	O	S	0	0
			1711	1109	279	315	8		

- Molecule 12 is a protein called Lhcb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	211	Total	C	N	O	S	0	0
			1606	1033	260	304	9		
12	9	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	6	219	Total	C	N	O	S	0	0
			1670	1073	271	317	9		
12	u	219	Total	C	N	O	S	0	0
			1683	1084	271	319	9		
12	p	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	7	219	Total	C	N	O	S	0	0
			1677	1080	271	317	9		

- Molecule 13 is a protein called LhcbS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		
13	s	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		

- Molecule 14 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	34	Total 226	C 146	N 36	O 44	0	0
14	x	34	Total 226	C 146	N 36	O 44	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	25	Total 179	C 118	N 30	O 31	0	0
15	v	25	Total 179	C 118	N 30	O 31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total 236	C 165	N 34	O 36	S 1	0	0
16	t	28	Total 236	C 165	N 34	O 36	S 1	0	0

- Molecule 17 is a protein called LhcbG.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	N	206	Total 1551	C 1002	N 247	O 292	S 10	0	0
17	Y	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	8	206	Total 1554	C 1005	N 247	O 292	S 10	0	0
17	g	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	n	206	Total 1545	C 998	N 247	O 290	S 10	0	0
17	y	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	q	206	Total 1554	C 1005	N 247	O 292	S 10	0	0

- Molecule 18 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		
18	b	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	SER	conflict	UNP A0A0D6E1D0
B	353	GLU	GLN	conflict	UNP A0A0D6E1D0
B	355	HIS	TYR	conflict	UNP A0A0D6E1D0
b	281	ALA	SER	conflict	UNP A0A0D6E1D0
b	353	GLU	GLN	conflict	UNP A0A0D6E1D0
b	355	HIS	TYR	conflict	UNP A0A0D6E1D0

- Molecule 19 is a protein called PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		
19	a	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		

- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		
20	c	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	MET	conflict	UNP D0EVT6
c	1	VAL	MET	conflict	UNP D0EVT6

- Molecule 21 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

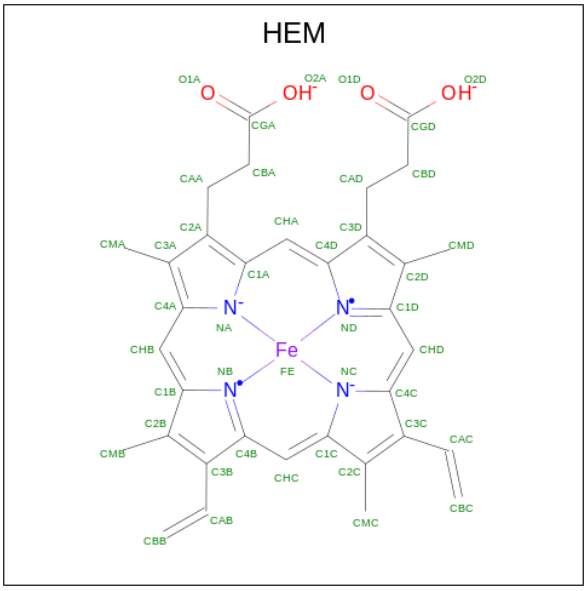
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ILE	VAL	conflict	UNP A0A0B5GKA5
d	55	ILE	VAL	conflict	UNP A0A0B5GKA5

- Molecule 22 is a protein called PsbW.

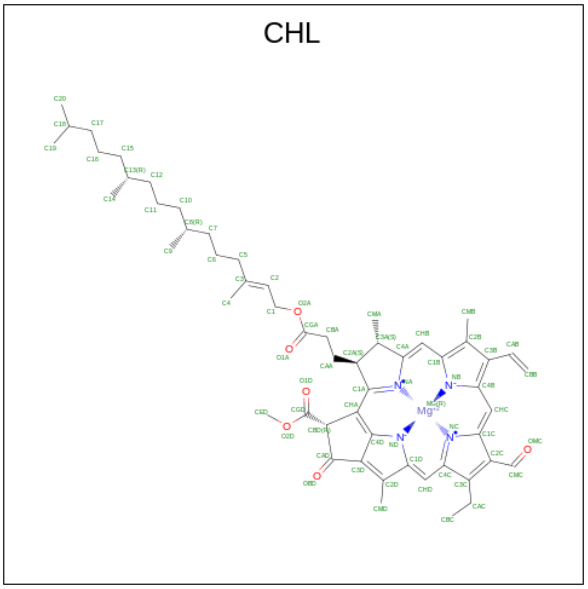
Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			304	191	49	64		
22	w	43	Total	C	N	O	0	0
			304	191	49	64		

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
23	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	G	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	N	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	Y	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	Y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	n	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	y	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

Continued on next page...

Continued from previous page...

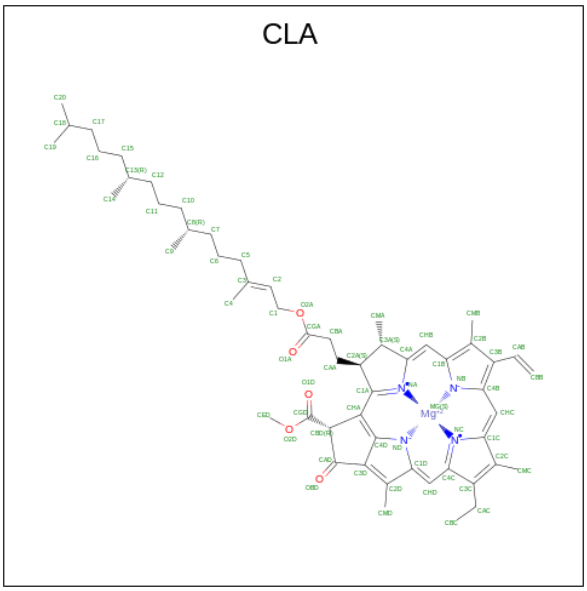
Mol	Chain	Residues	Atoms					AltConf
24	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	Y	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	y	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

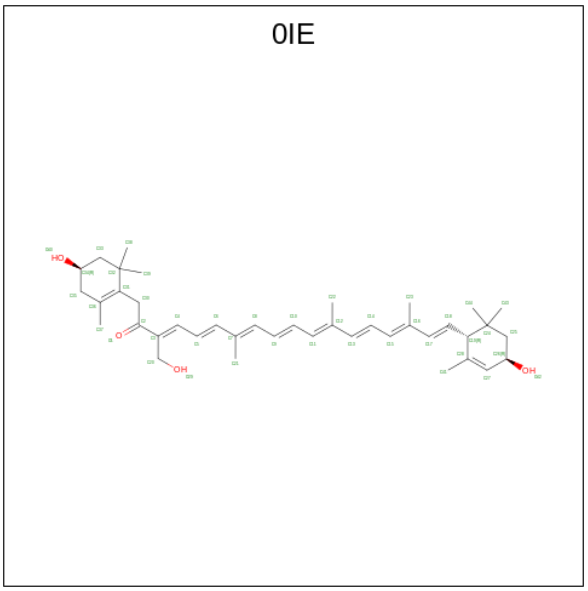
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	r	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	7	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	7	1	Total 52	C 42	Mg 1	N 4	O 5	0

- Molecule 26 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



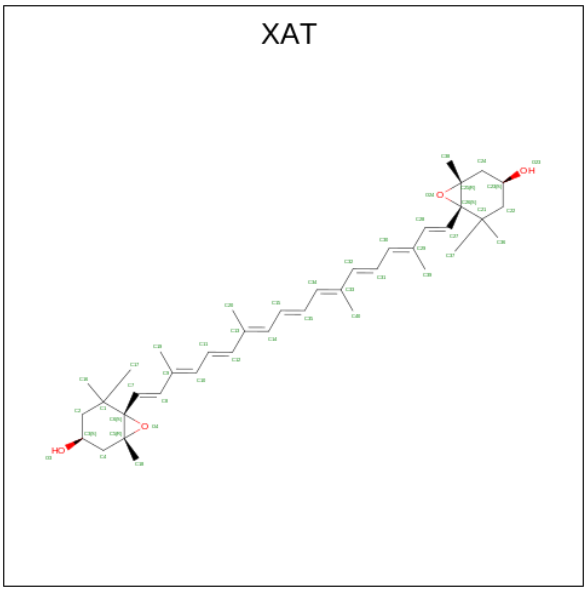
Mol	Chain	Residues	Atoms	AltConf
26	R	1	Total C O 44 40 4	0
26	1	1	Total C O 44 40 4	0
26	2	1	Total C O 44 40 4	0
26	2	1	Total C O 44 40 4	0
26	3	1	Total C O 43 39 4	0
26	3	1	Total C O 44 40 4	0
26	G	1	Total C O 44 40 4	0
26	G	1	Total C O 44 40 4	0
26	9	1	Total C O 44 40 4	0
26	9	1	Total C O 44 40 4	0
26	N	1	Total C O 44 40 4	0
26	Y	1	Total C O 44 40 4	0
26	Y	1	Total C O 44 40 4	0
26	8	1	Total C O 44 40 4	0

Continued on next page...

Continued from previous page...

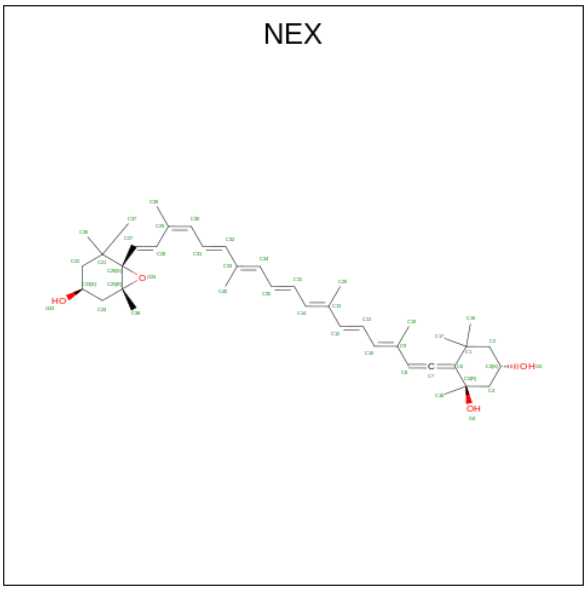
Mol	Chain	Residues	Atoms	AltConf
26	4	1	Total C O 44 40 4	0
26	5	1	Total C O 44 40 4	0
26	5	1	Total C O 44 40 4	0
26	6	1	Total C O 43 39 4	0
26	g	1	Total C O 44 40 4	0
26	g	1	Total C O 44 40 4	0
26	u	1	Total C O 44 40 4	0
26	u	1	Total C O 44 40 4	0
26	n	1	Total C O 44 40 4	0
26	y	1	Total C O 44 40 4	0
26	y	1	Total C O 44 40 4	0
26	p	1	Total C O 44 40 4	0
26	p	1	Total C O 44 40 4	0
26	q	1	Total C O 44 40 4	0
26	r	1	Total C O 44 40 4	0
26	7	1	Total C O 44 40 4	0
26	7	1	Total C O 44 40 4	0

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



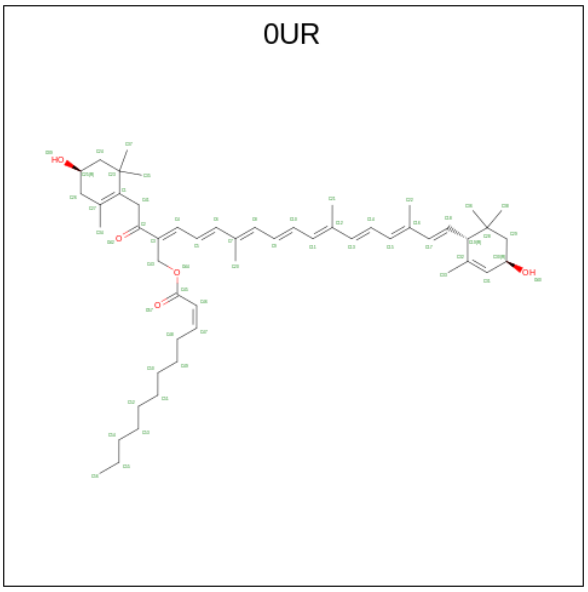
Mol	Chain	Residues	Atoms			AltConf
27	R	1	Total 44	C 40	O 4	0
27	r	1	Total 44	C 40	O 4	0

- Molecule 28 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
28	R	1	Total C O 44 40 4	0
28	1	1	Total C O 44 40 4	0
28	2	1	Total C O 44 40 4	0
28	3	1	Total C O 44 40 4	0
28	S	1	Total C O 44 40 4	0
28	G	1	Total C O 44 40 4	0
28	9	1	Total C O 44 40 4	0
28	N	1	Total C O 44 40 4	0
28	4	1	Total C O 44 40 4	0
28	5	1	Total C O 44 40 4	0
28	6	1	Total C O 44 40 4	0
28	g	1	Total C O 44 40 4	0
28	u	1	Total C O 44 40 4	0
28	n	1	Total C O 44 40 4	0
28	y	1	Total C O 44 40 4	0
28	p	1	Total C O 44 40 4	0
28	s	1	Total C O 44 40 4	0
28	r	1	Total C O 44 40 4	0
28	r	1	Total C O 44 40 4	0
28	7	1	Total C O 44 40 4	0

- Molecule 29 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



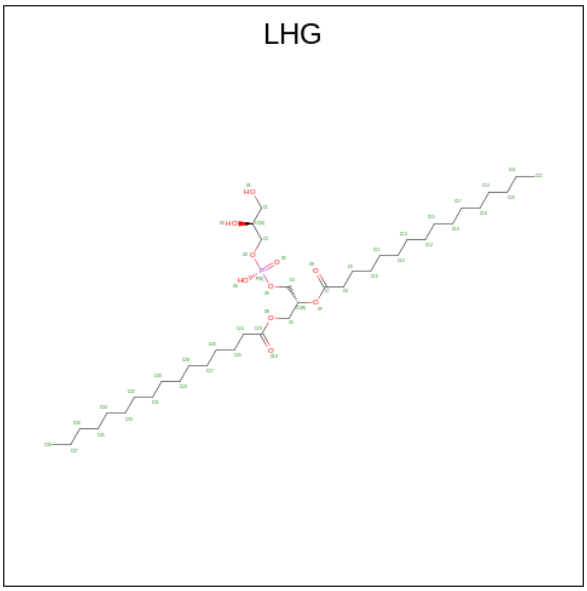
Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O 52 47 5	0
29	2	1	Total C O 52 47 5	0
29	3	1	Total C O 52 47 5	0
29	G	1	Total C O 52 47 5	0
29	9	1	Total C O 52 47 5	0
29	N	1	Total C O 52 47 5	0
29	Y	1	Total C O 52 47 5	0
29	8	1	Total C O 52 47 5	0
29	4	1	Total C O 52 47 5	0
29	5	1	Total C O 52 47 5	0
29	6	1	Total C O 52 47 5	0
29	g	1	Total C O 52 47 5	0
29	u	1	Total C O 52 47 5	0
29	n	1	Total C O 52 47 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
29	y	1	Total C O 52 47 5	0
29	p	1	Total C O 52 47 5	0
29	q	1	Total C O 52 47 5	0
29	7	1	Total C O 52 47 5	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



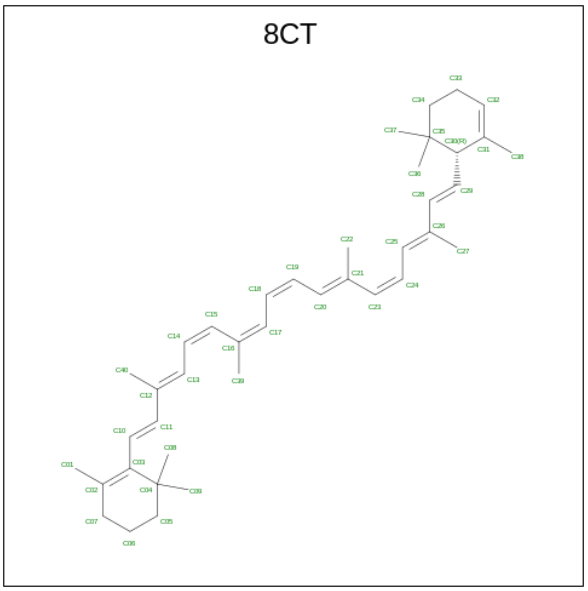
Mol	Chain	Residues	Atoms	AltConf
30	1	1	Total C O P 42 31 10 1	0
30	2	1	Total C O P 40 29 10 1	0
30	G	1	Total C O P 43 32 10 1	0
30	9	1	Total C O P 43 32 10 1	0
30	N	1	Total C O P 43 32 10 1	0
30	Y	1	Total C O P 43 32 10 1	0
30	A	1	Total C O P 45 34 10 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			44	33	10	1	
30	C	1	Total	C	O	P	0
			32	21	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	
30	4	1	Total	C	O	P	0
			42	31	10	1	
30	5	1	Total	C	O	P	0
			43	32	10	1	
30	g	1	Total	C	O	P	0
			43	32	10	1	
30	n	1	Total	C	O	P	0
			43	32	10	1	
30	y	1	Total	C	O	P	0
			43	32	10	1	
30	p	1	Total	C	O	P	0
			43	32	10	1	
30	a	1	Total	C	O	P	0
			45	34	10	1	
30	a	1	Total	C	O	P	0
			44	33	10	1	
30	c	1	Total	C	O	P	0
			32	21	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			39	28	10	1	
30	7	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 31 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



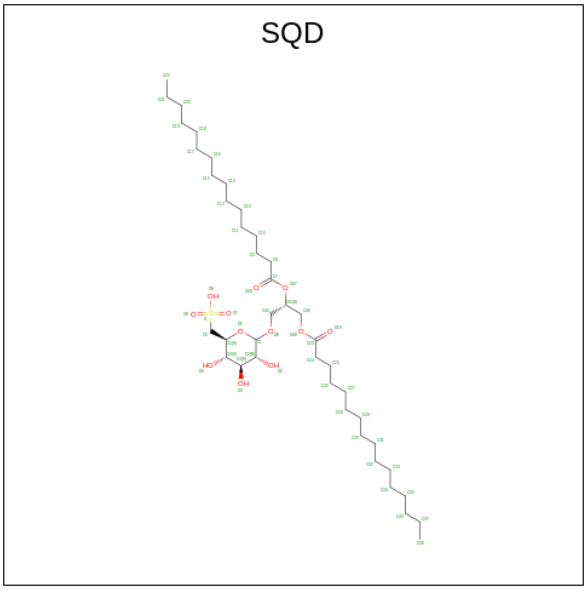
Mol	Chain	Residues	Atoms	AltConf
31	S	1	Total C 40 40	0
31	S	1	Total C 40 40	0
31	X	1	Total C 40 40	0
31	V	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	x	1	Total C 40 40	0
31	v	1	Total C 40 40	0
31	t	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



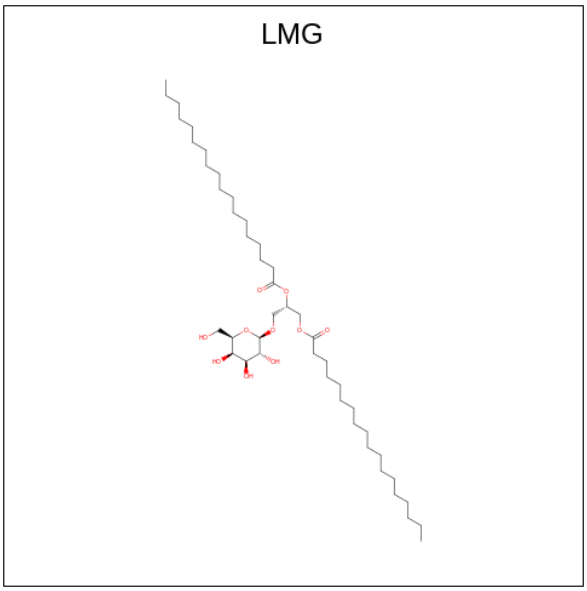
Mol	Chain	Residues	Atoms	AltConf
32	B	1	Total C O S 54 41 12 1	0
32	A	1	Total C O S 45 32 12 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	S	0
			44	31	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			45	32	12	1	
32	d	1	Total	C	O	S	0
			44	31	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



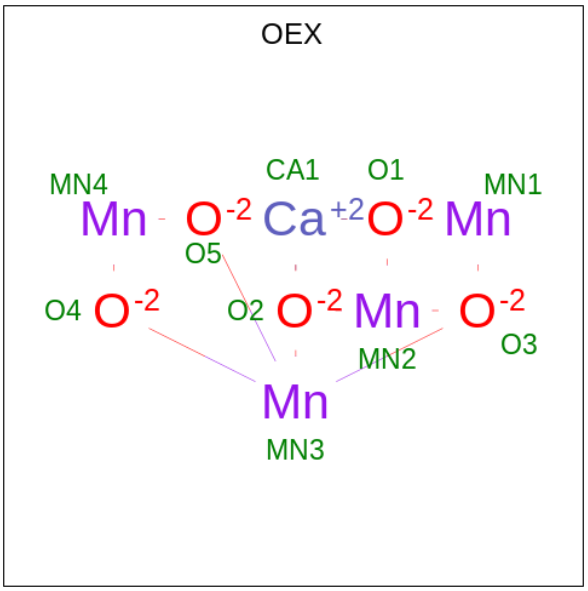
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			41	31	10	
33	C	1	Total	C	O	0
			42	32	10	
33	D	1	Total	C	O	0
			48	38	10	
33	D	1	Total	C	O	0
			46	36	10	
33	W	1	Total	C	O	0
			30	20	10	
33	i	1	Total	C	O	0
			48	38	10	
33	m	1	Total	C	O	0
			41	31	10	

Continued on next page...

Continued from previous page...

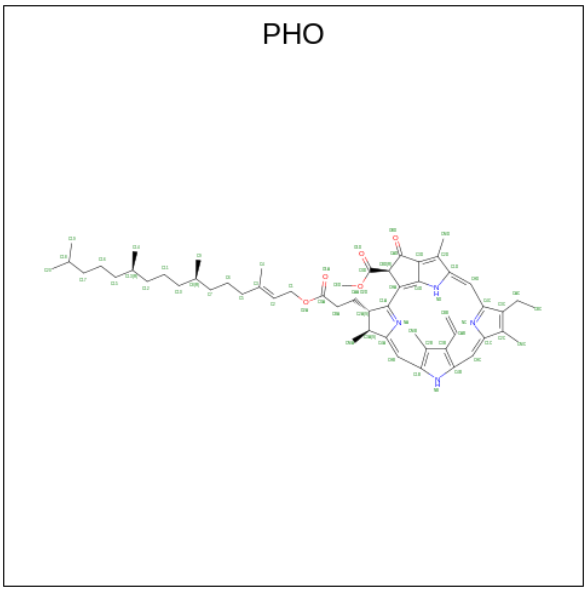
Mol	Chain	Residues	Atoms			AltConf
33	w	1	Total 36	C 26	O 10	0
33	d	1	Total 48	C 38	O 10	0
33	d	1	Total 46	C 36	O 10	0

- Molecule 34 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



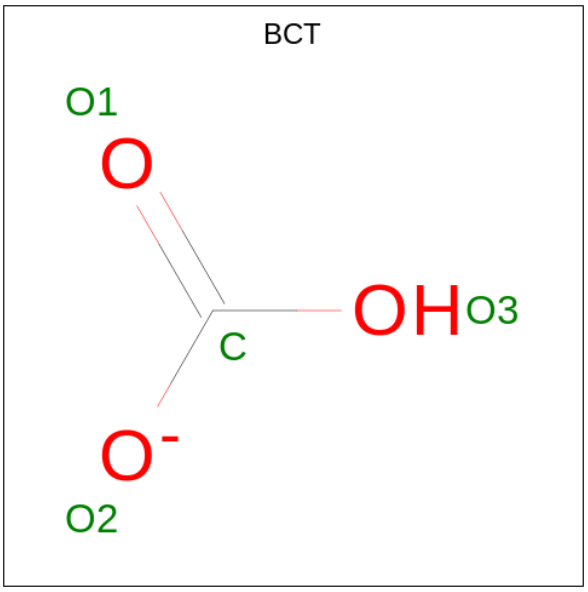
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total 10	Ca 1	Mn 4	O 5	0
34	a	1	Total 10	Ca 1	Mn 4	O 5	0

- Molecule 35 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



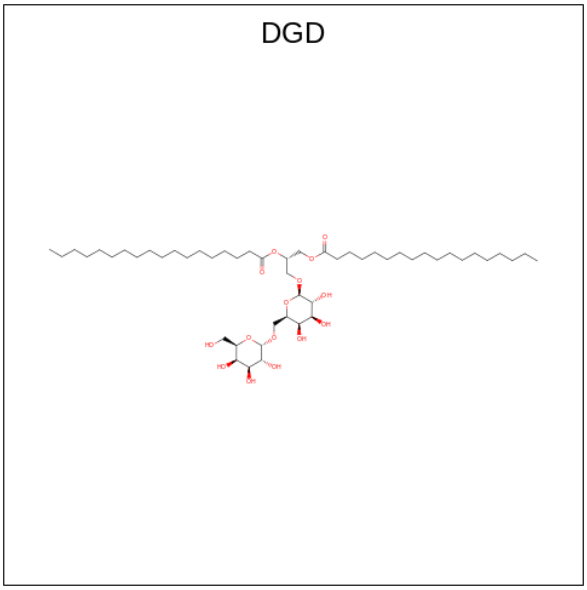
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			64	55	4	5	
35	D	1	Total	C	N	O	0
			64	55	4	5	
35	a	1	Total	C	N	O	0
			64	55	4	5	
35	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C O 4 1 3	0
36	a	1	Total C O 4 1 3	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

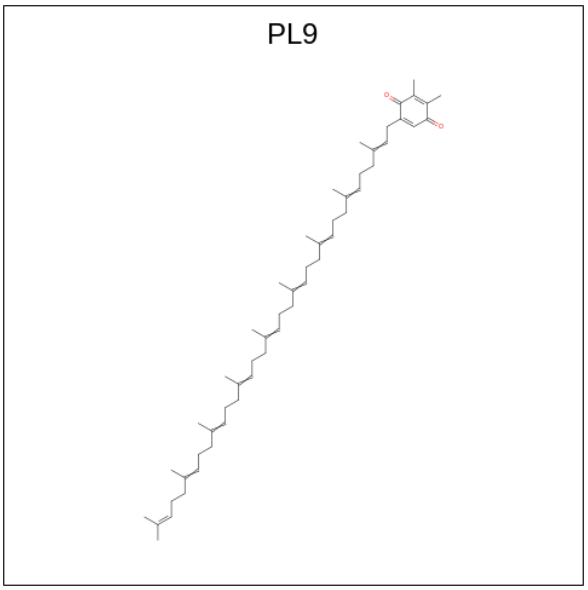


Mol	Chain	Residues	Atoms	AltConf
37	C	1	Total C O 50 35 15	0
37	C	1	Total C O 55 40 15	0
37	c	1	Total C O 50 35 15	0
37	c	1	Total C O 55 40 15	0

- Molecule 38 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
38	D	1	Total Fe 1 1	0
38	d	1	Total Fe 1 1	0

- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
39	D	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	

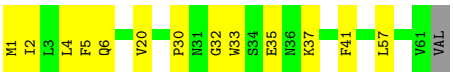
3 Residue-property plots (i)

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 II reaction center protein Z

Chain Z:





• Molecule 1: Photosystem II reaction center protein Z

Chain z:

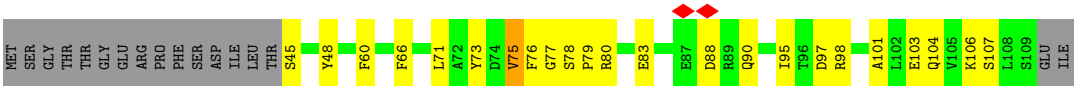




• Molecule 2: Cytochrome b559 subunit alpha

Chain E:





• Molecule 2: Cytochrome b559 subunit alpha

Chain e:

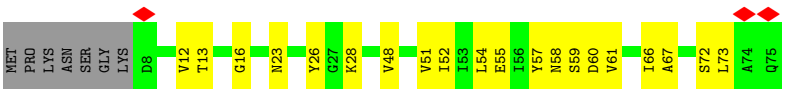




• Molecule 3: Photosystem II reaction center protein H

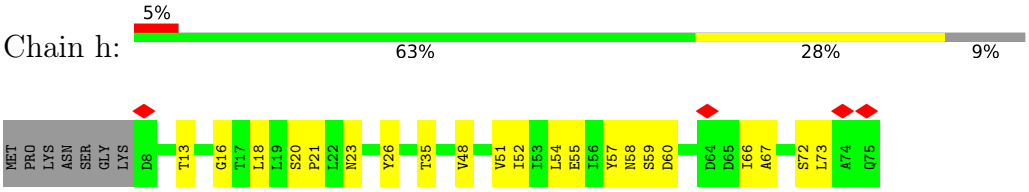
Chain H:





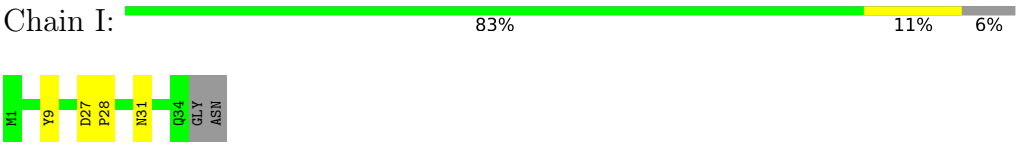
• Molecule 3: Photosystem II reaction center protein H

Chain h:



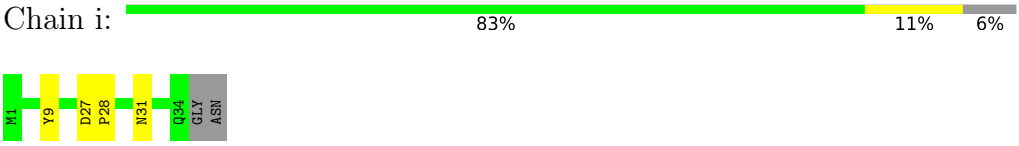
• Molecule 4: Photosystem II reaction center protein I

Chain I:



• Molecule 4: Photosystem II reaction center protein I

Chain i:



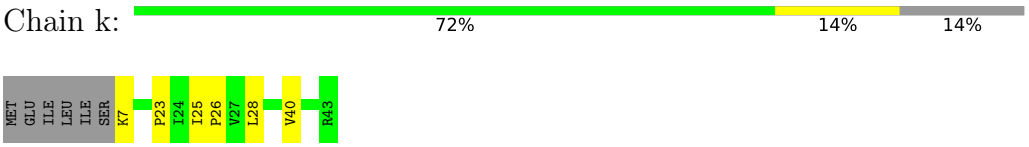
• Molecule 5: Photosystem II reaction center protein K

Chain K:



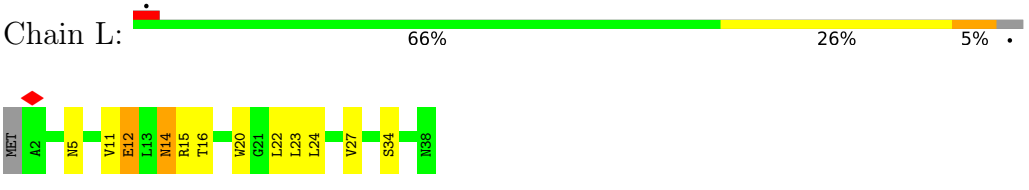
• Molecule 5: Photosystem II reaction center protein K

Chain k:



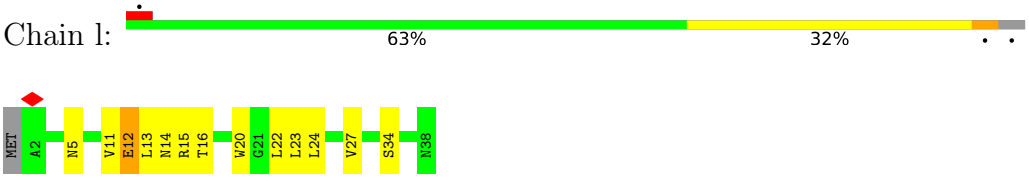
• Molecule 6: Photosystem II reaction center protein L

Chain L:

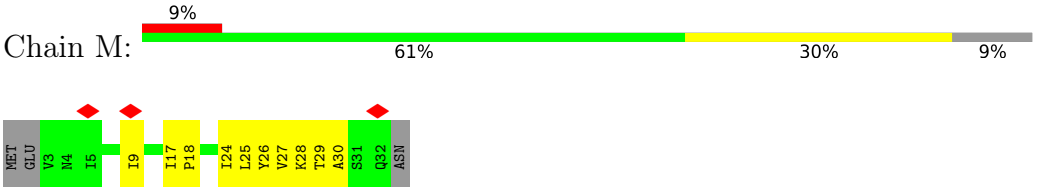


• Molecule 6: Photosystem II reaction center protein L

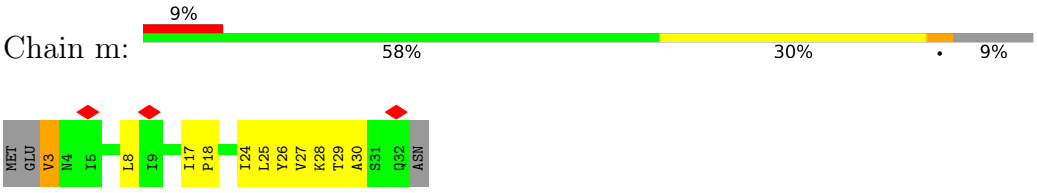
Chain l:



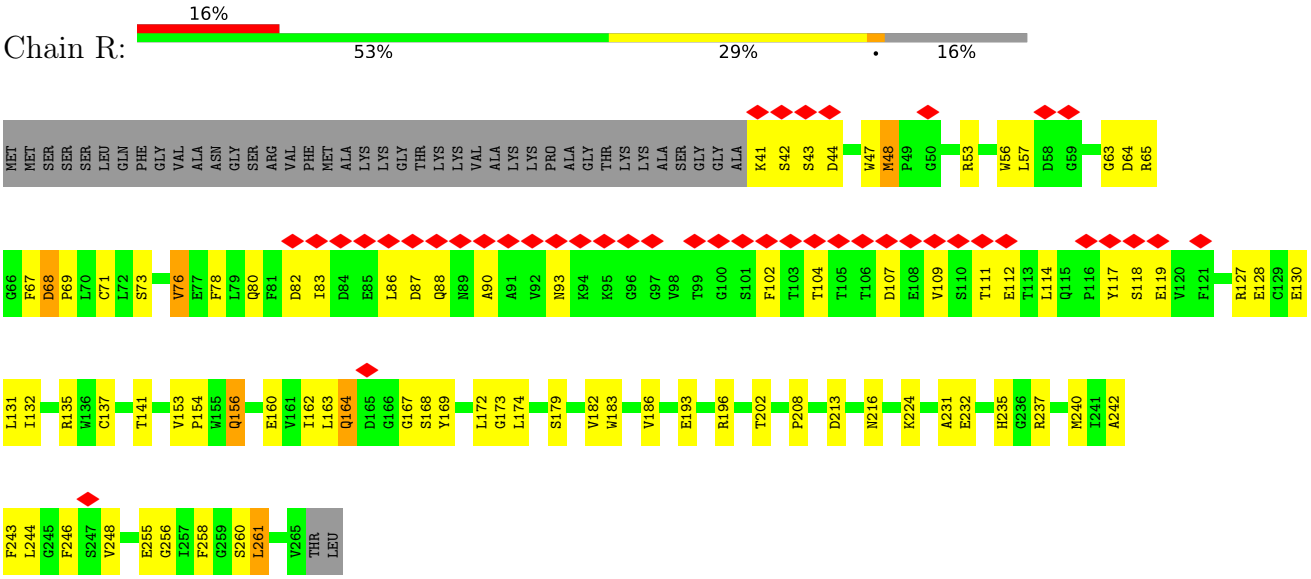
• Molecule 7: Photosystem II reaction center protein M



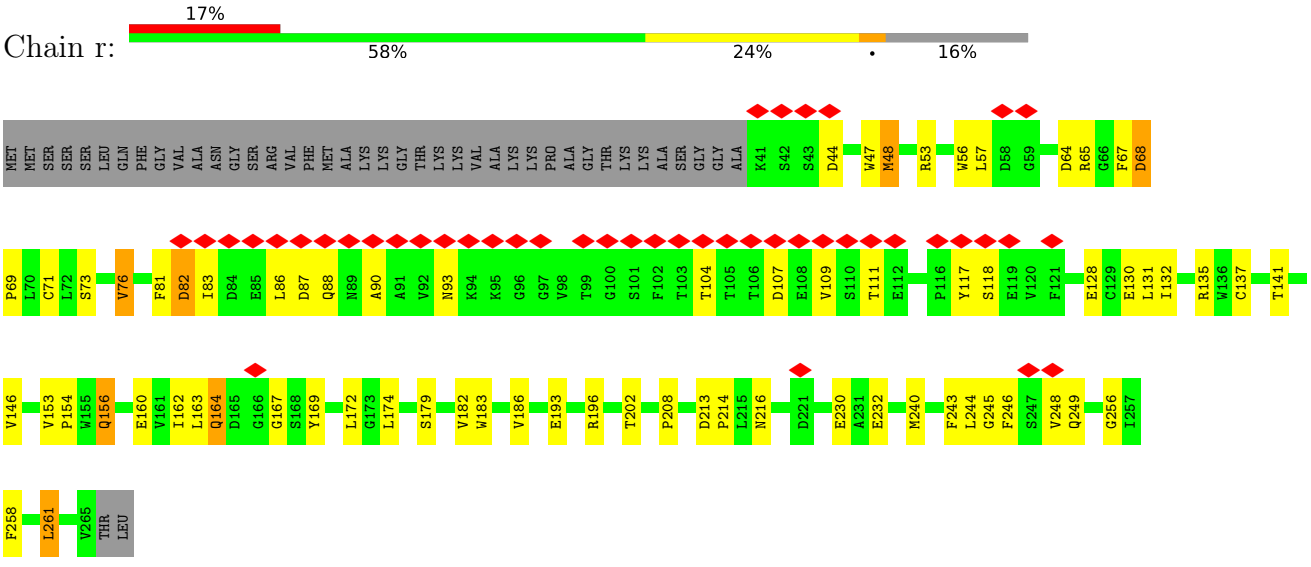
• Molecule 7: Photosystem II reaction center protein M



• Molecule 8: PsbR



• Molecule 8: PsbR



• Molecule 9: Cytochrome b559 subunit beta

Chain F:



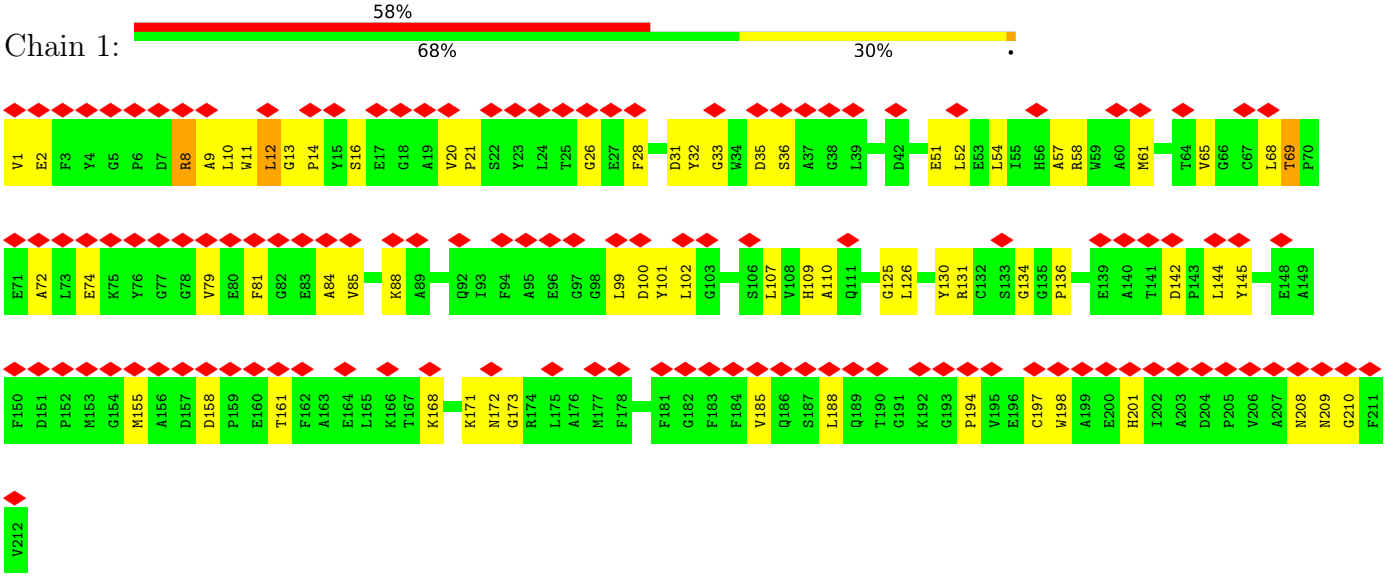
• Molecule 9: Cytochrome b559 subunit beta

Chain f:



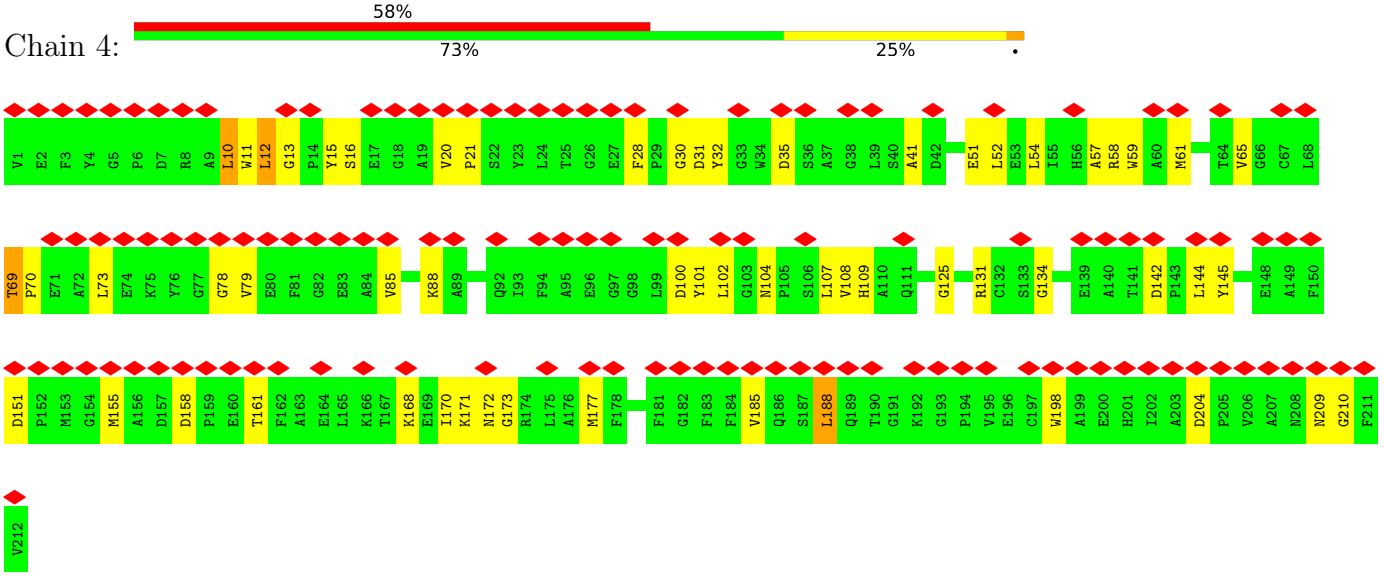
• Molecule 10: Lhcb1

Chain 1:



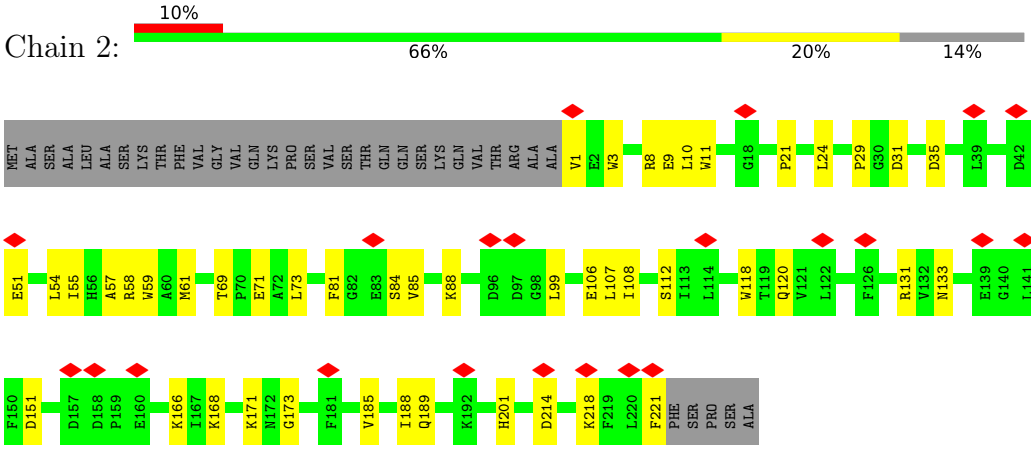
• Molecule 10: Lhcb1

Chain 4:



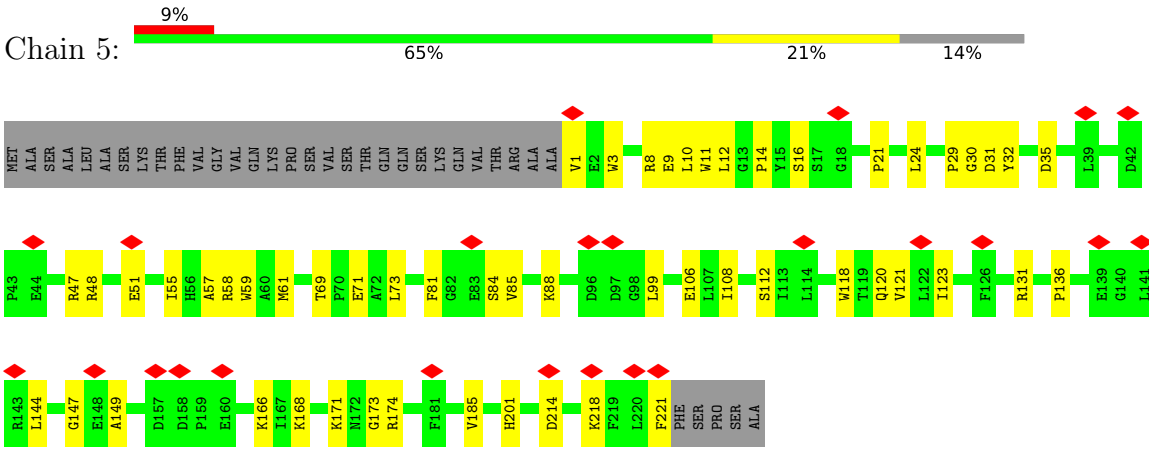
• Molecule 11: Lhcb2

Chain 2:



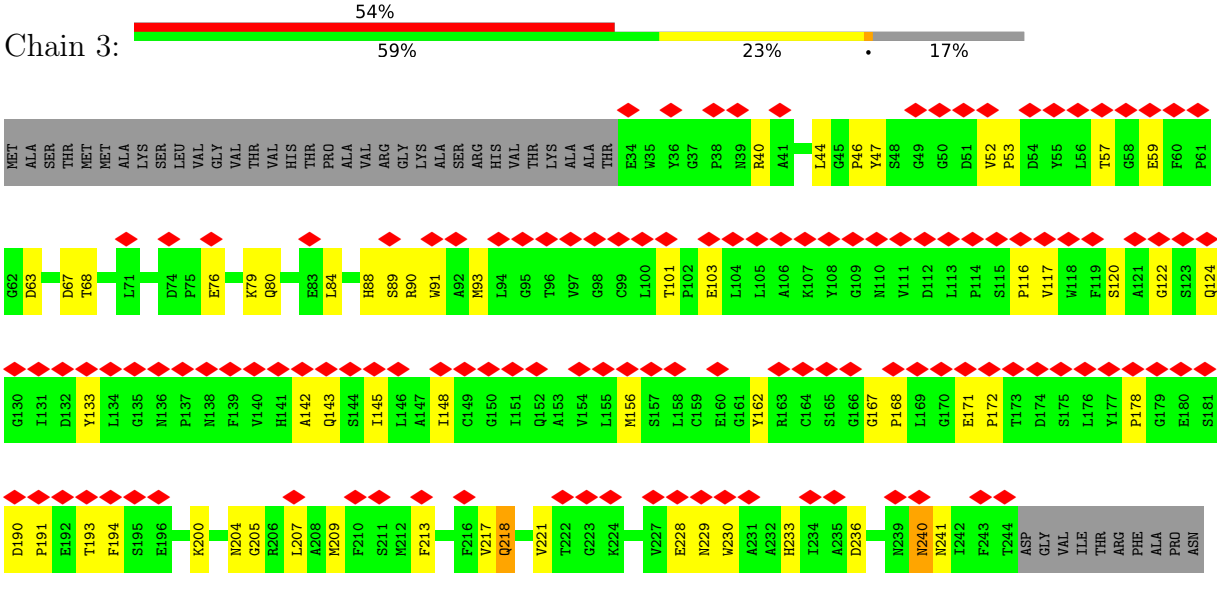
• Molecule 11: Lhcb2

Chain 5:



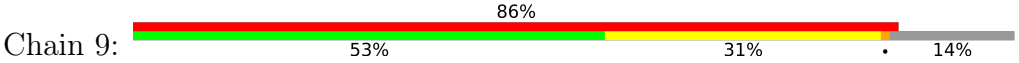
• Molecule 12: Lhcb3

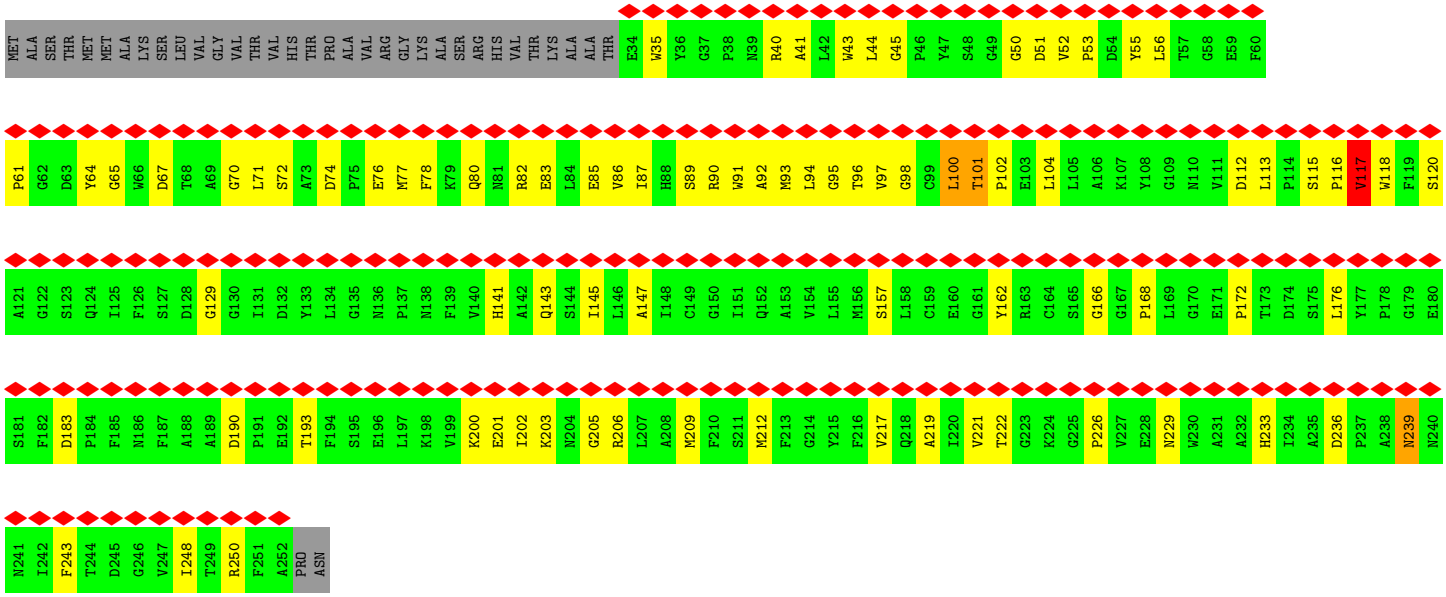
Chain 3:



• Molecule 12: Lhcb3

Chain 9:

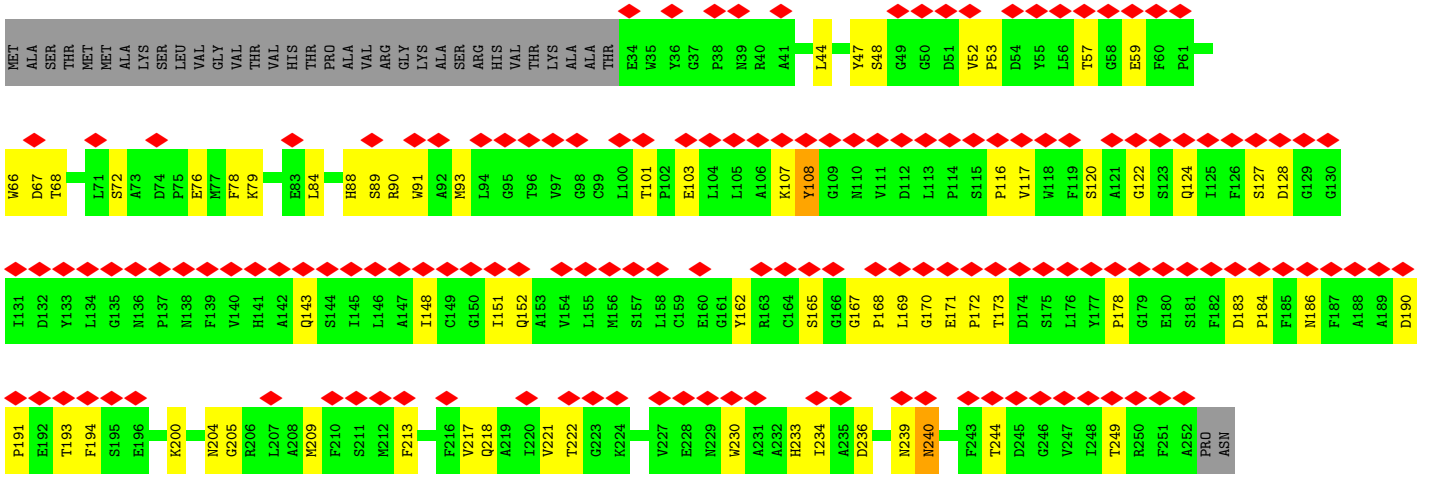




• Molecule 12: Lhcb3

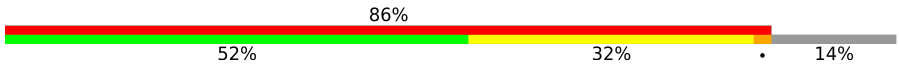
Chain 6:

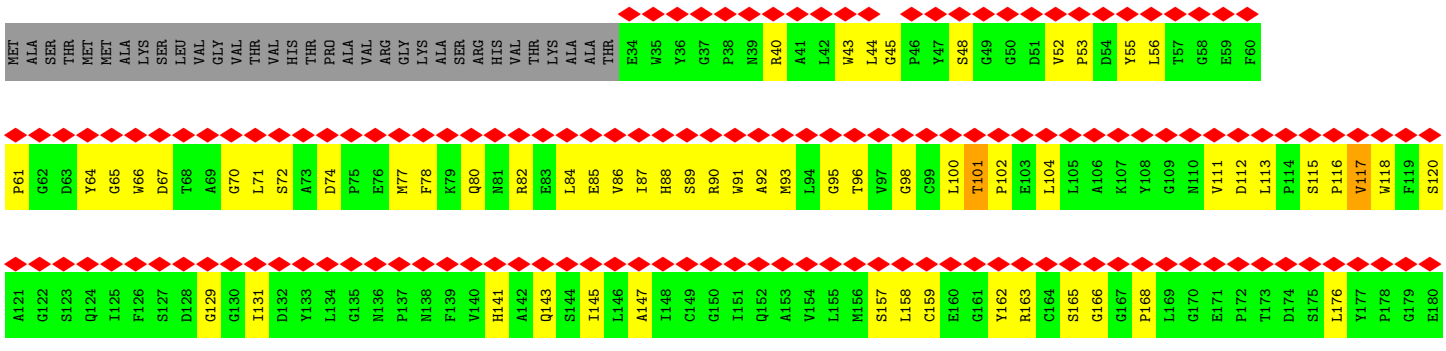


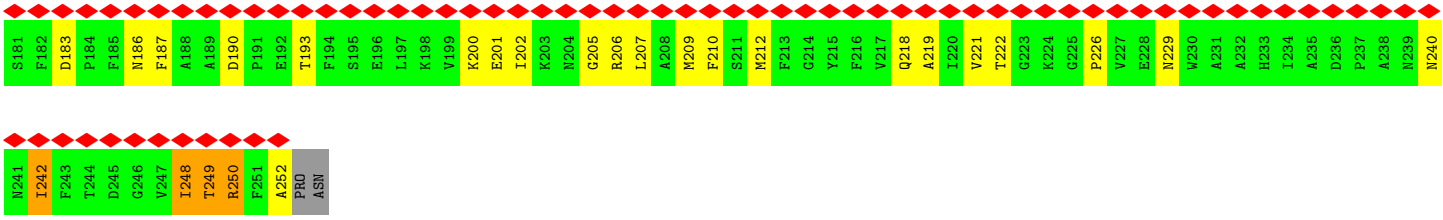


• Molecule 12: Lhcb3

Chain u:



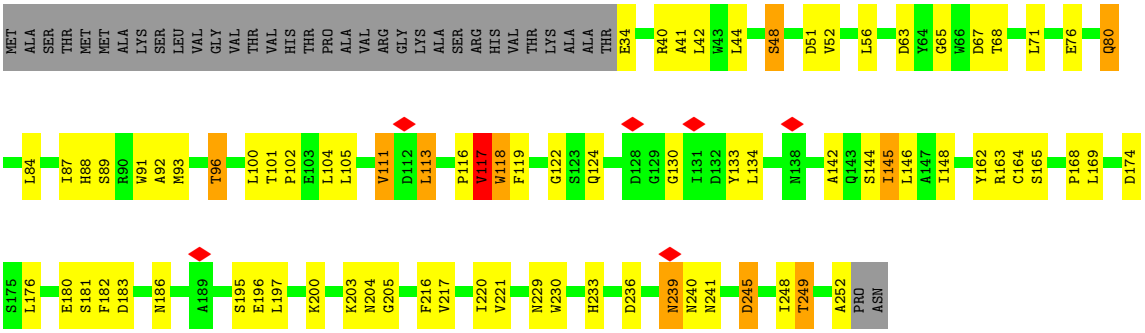




• Molecule 12: Lhcb3

Chain p:

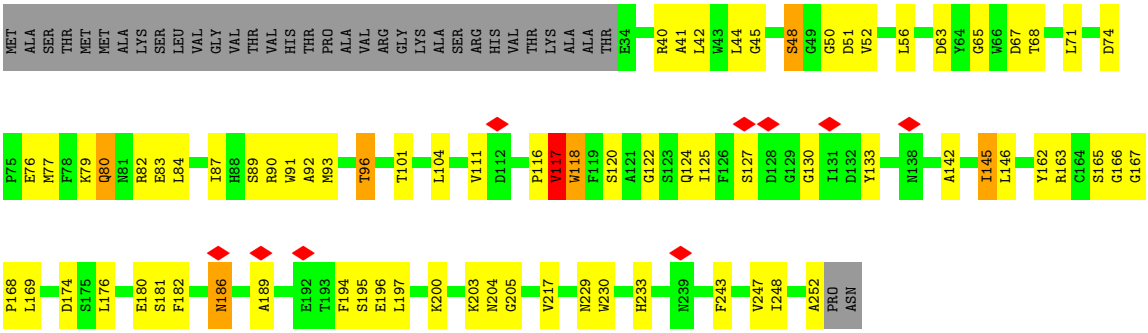




• Molecule 12: Lhcb3

Chain 7:

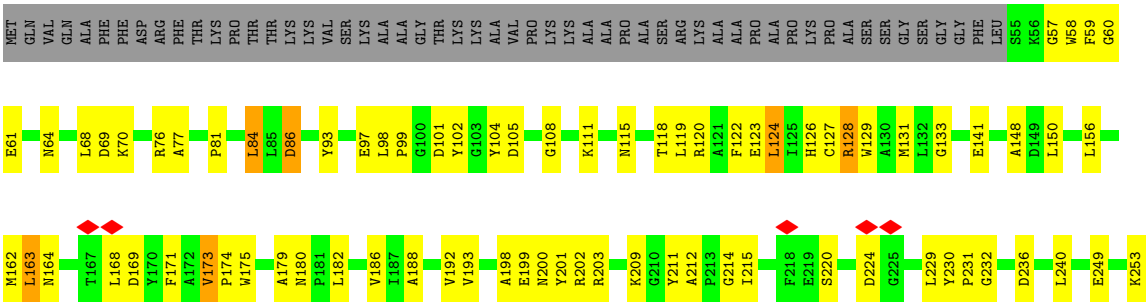


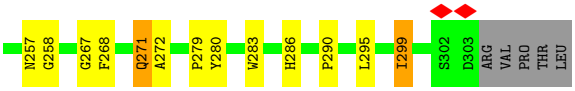


• Molecule 13: LhcbS

Chain S:



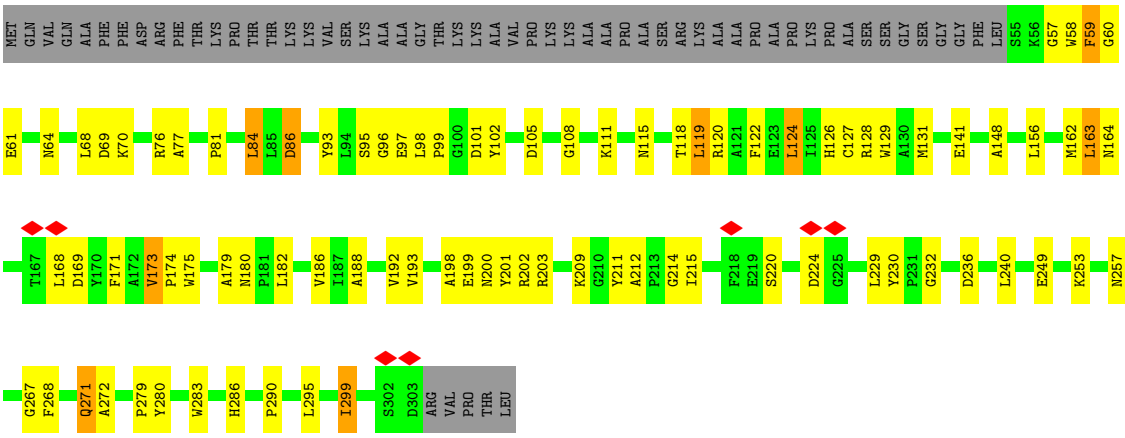




• Molecule 13: LhcbS

Chain s:

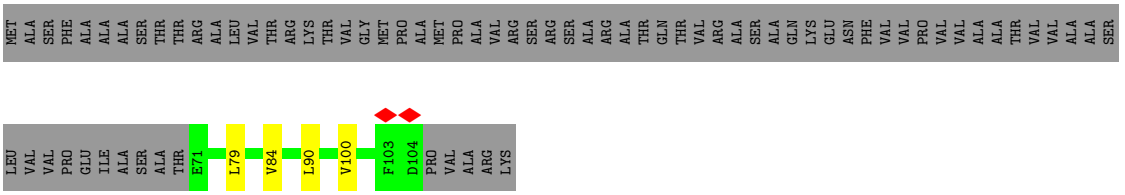




• Molecule 14: PsbX

Chain X:

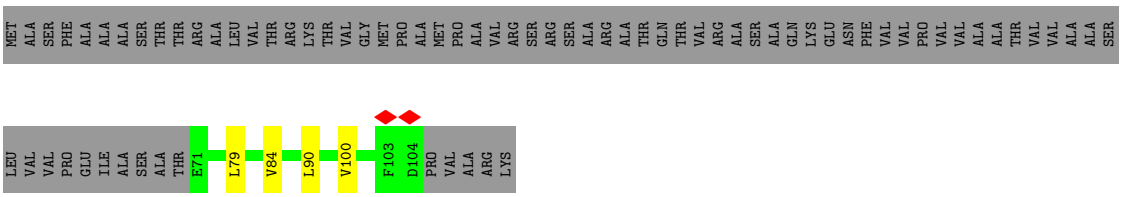




• Molecule 14: PsbX

Chain x:

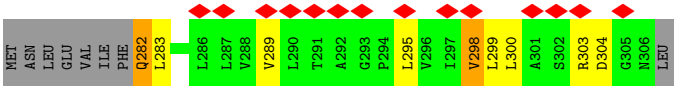




• Molecule 15: Photosystem II reaction center protein Psb30

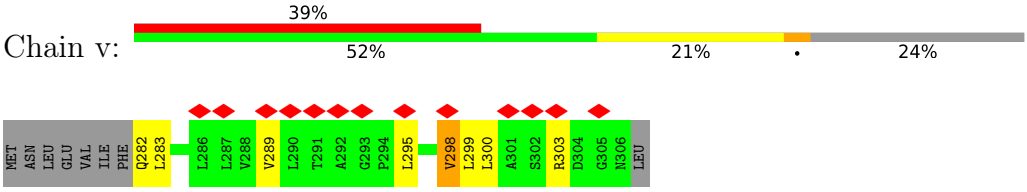
Chain V:





• Molecule 15: Photosystem II reaction center protein Psb30

Chain v:



• Molecule 16: Photosystem II reaction center protein T

Chain T:



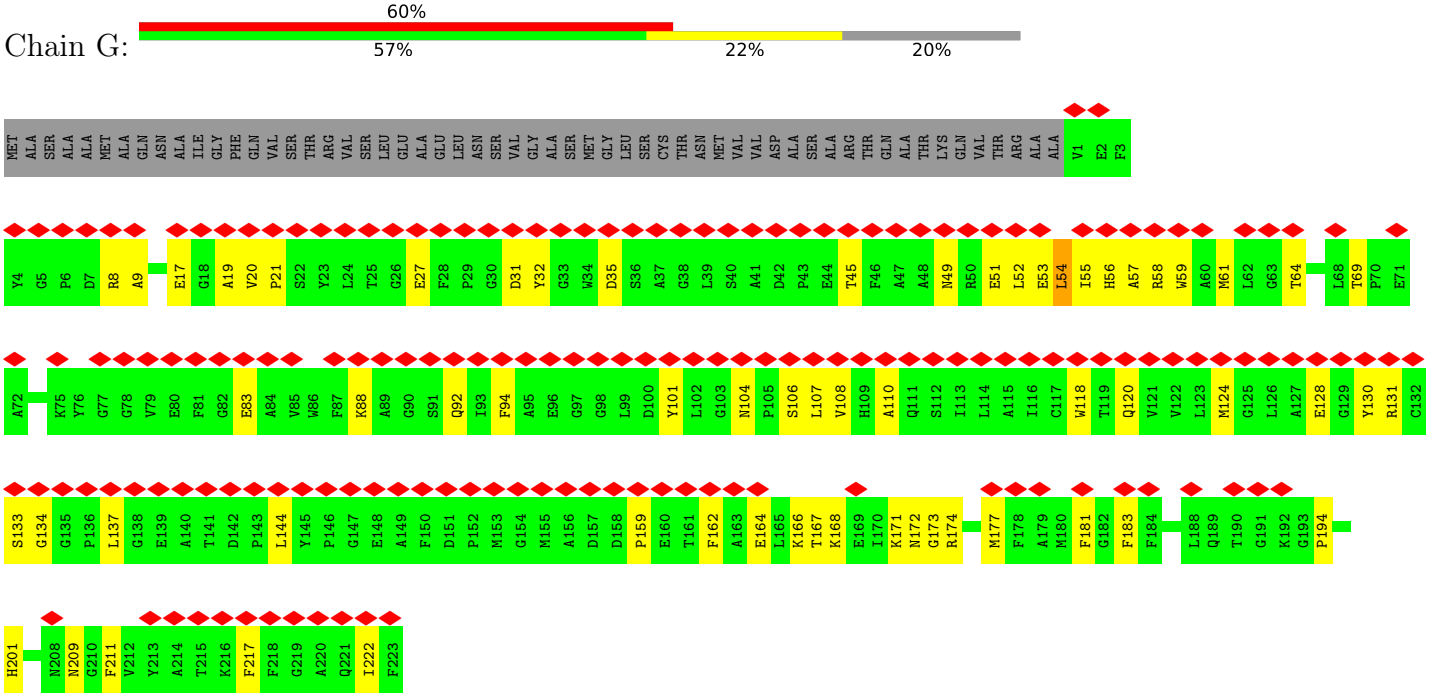
• Molecule 16: Photosystem II reaction center protein T

Chain t:



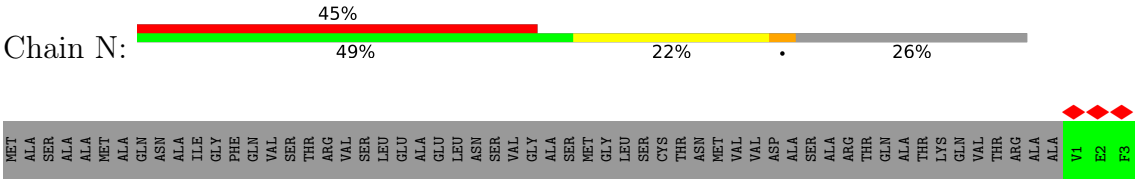
• Molecule 17: LhcbG

Chain G:



• Molecule 17: LhcbG

Chain N:

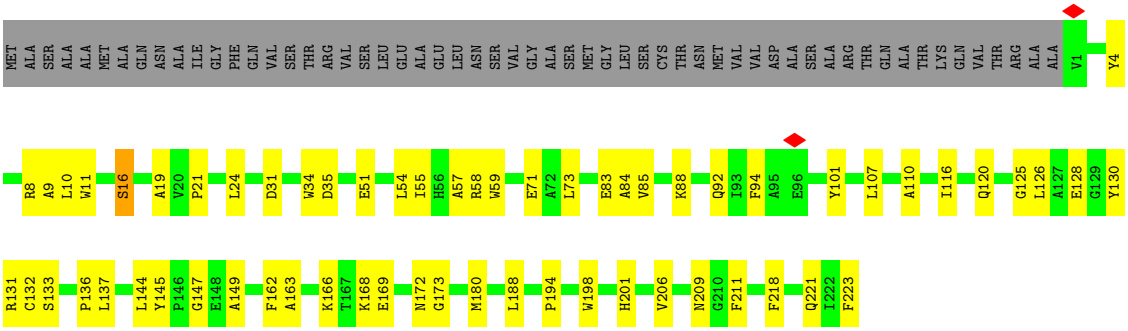




• Molecule 17: LhcbG

Chain Y:

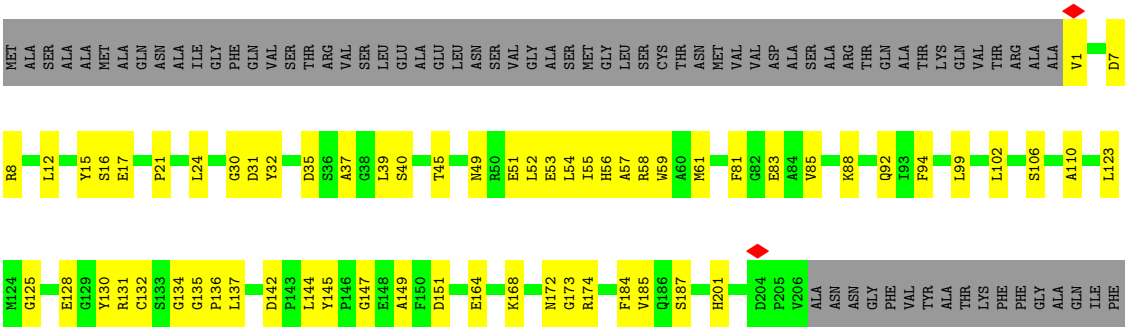




• Molecule 17: LhcbG

Chain 8:

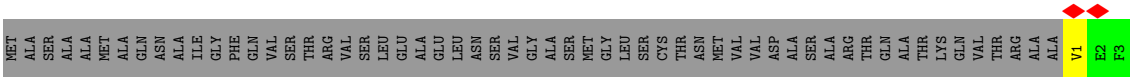




• Molecule 17: LhcbG

Chain g:



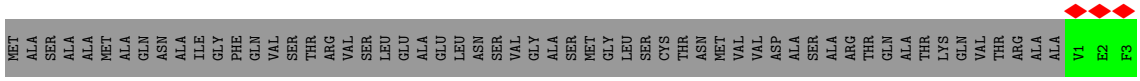


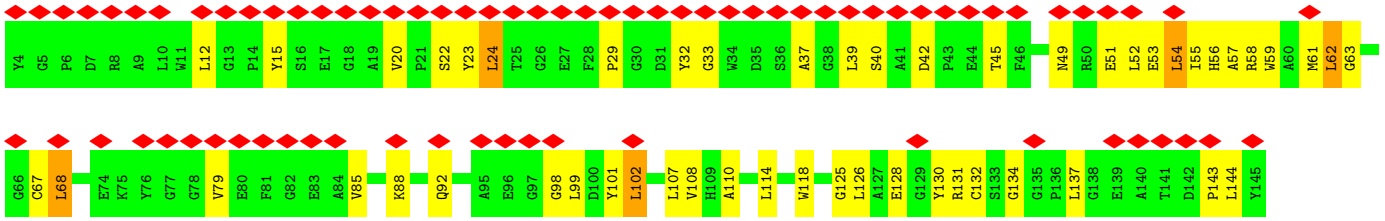


• Molecule 17: LhcbG

Chain n:



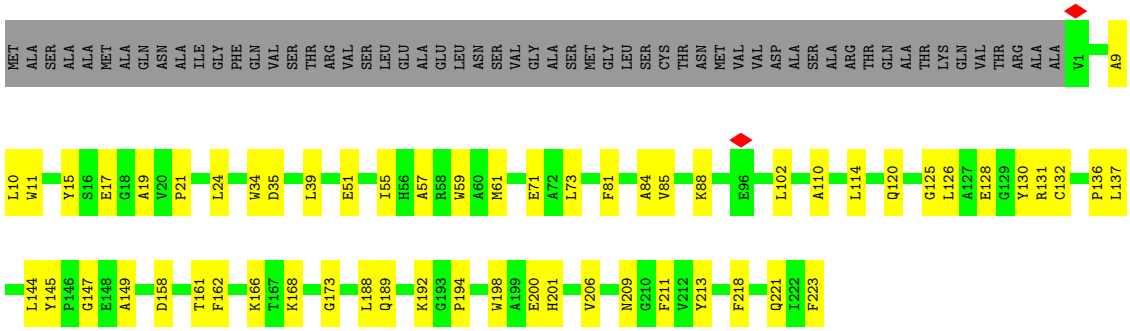




• Molecule 17: LhcbG

Chain y:

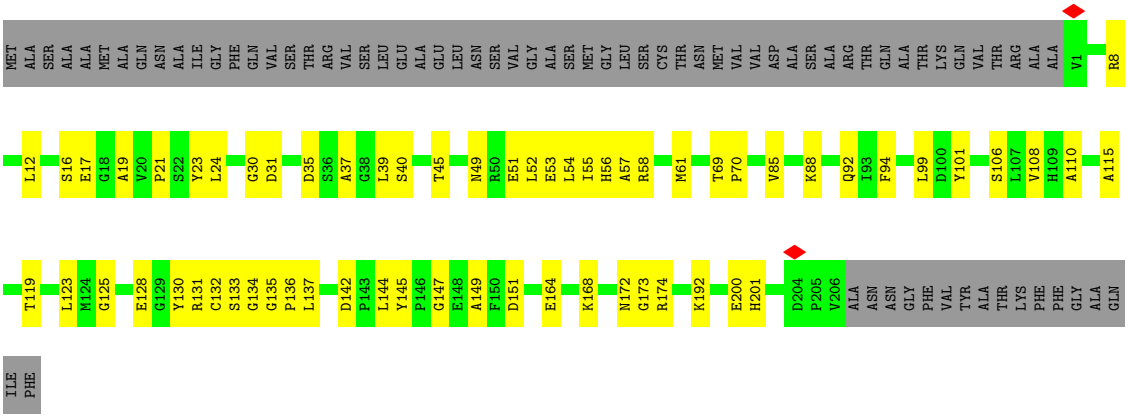




• Molecule 17: LhcbG

Chain q:

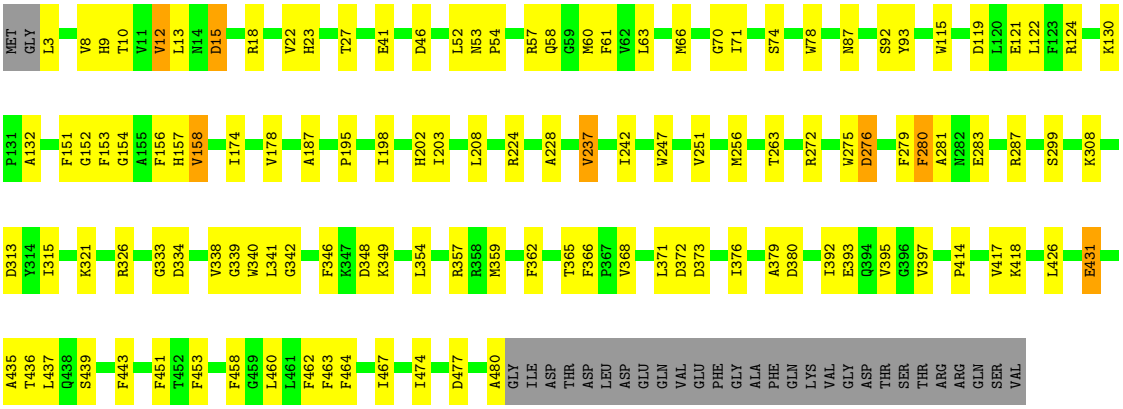




• Molecule 18: Photosystem II CP47 reaction center protein

Chain B:

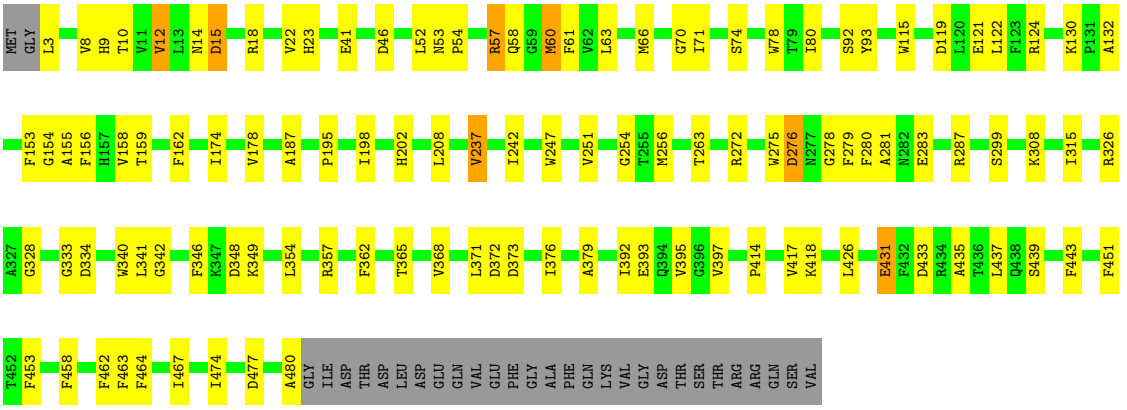




• Molecule 18: Photosystem II CP47 reaction center protein

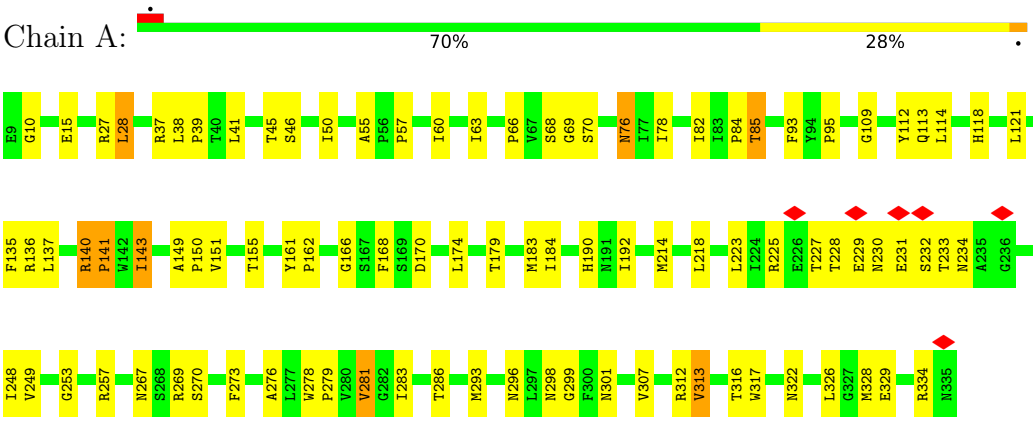
Chain b:





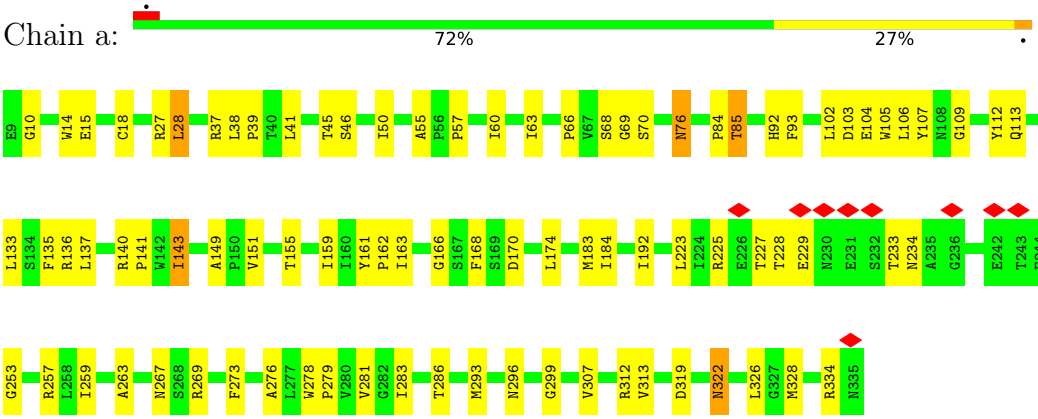
• Molecule 19: PsbA

Chain A:



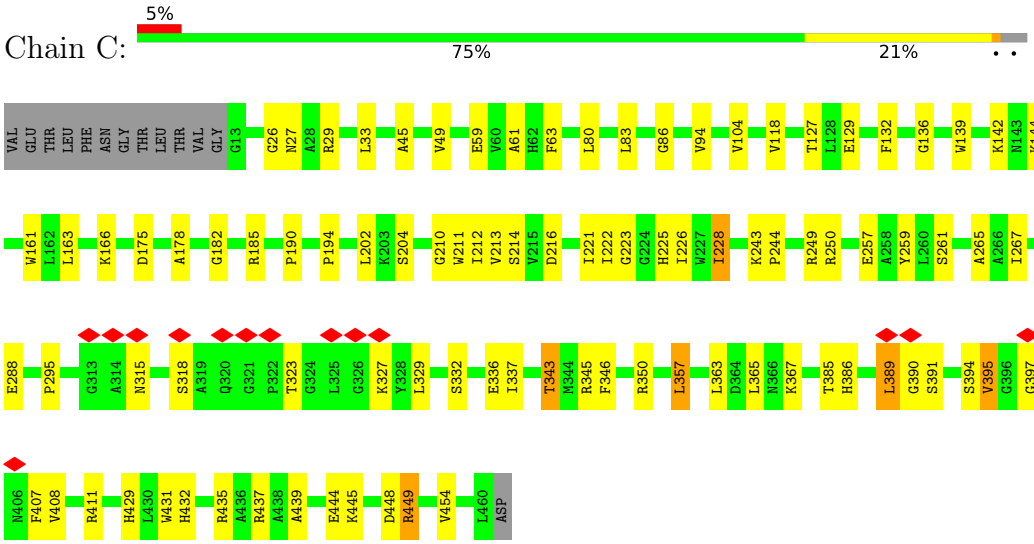
• Molecule 19: PsbA

Chain a:



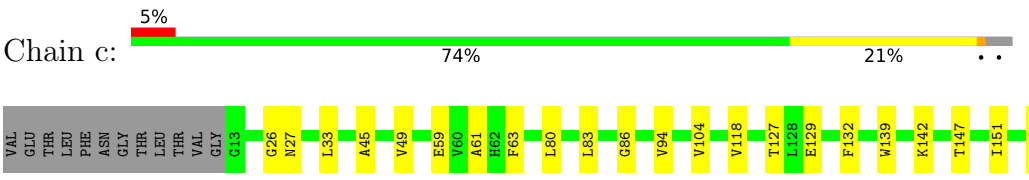
• Molecule 20: Photosystem II CP43 reaction center protein

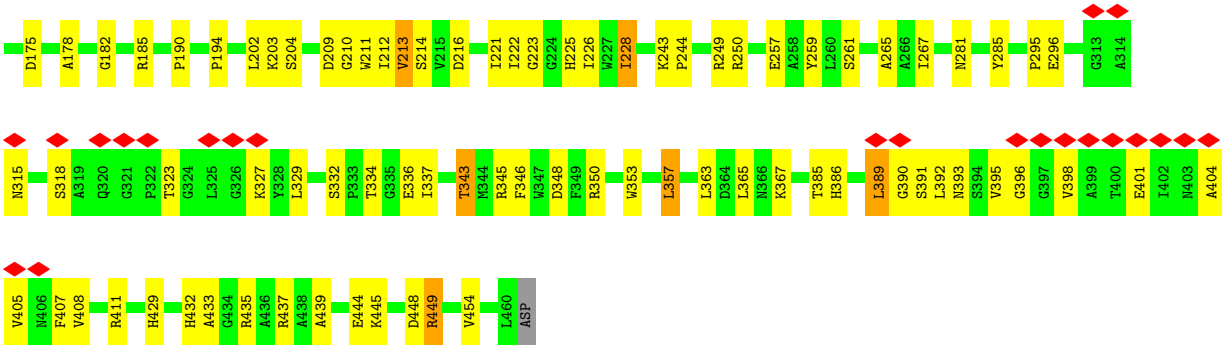
Chain C:



• Molecule 20: Photosystem II CP43 reaction center protein

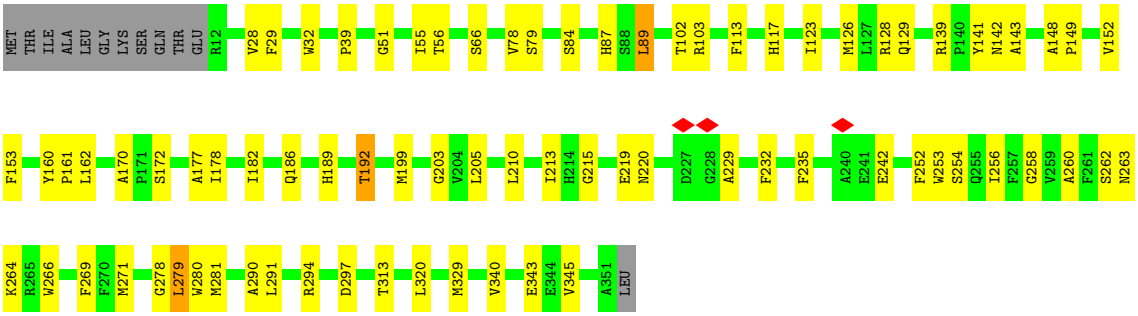
Chain c:





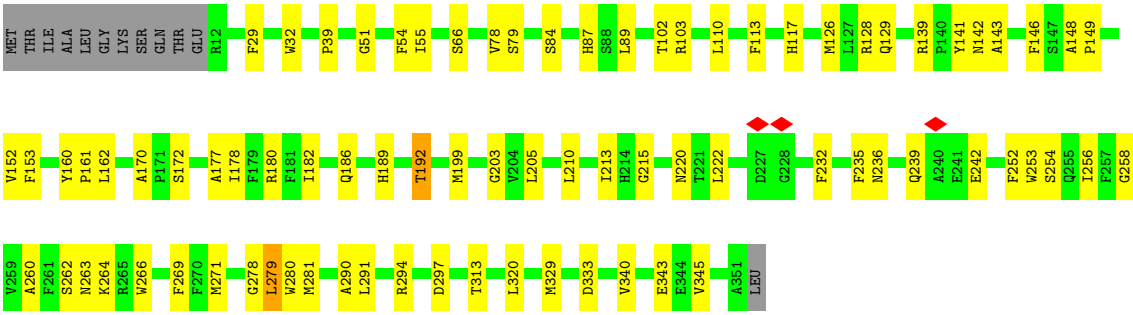
• Molecule 21: Photosystem II D2 protein





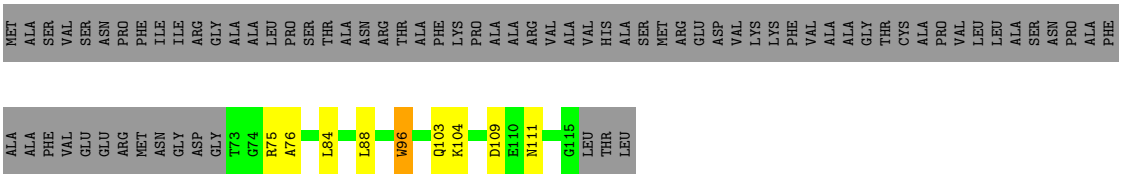
• Molecule 21: Photosystem II D2 protein





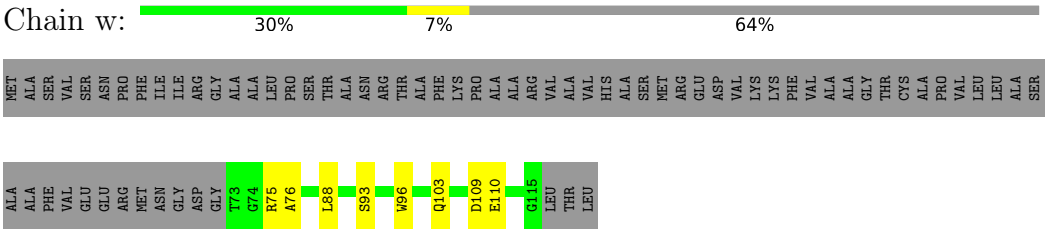
• Molecule 22: PsbW





• Molecule 22: PsbW

Chain w:


30%
7%
64%
MET ALA SER VAL SER ASN PRO PHE ILE ILE ARG GLY ALA ALA LEU PRO SER THR ALA ASN ARG THR ALA PHE LYS PRO ALA ALA ARG VAL ALA VAL HIS ALA SER MET ARG GLU ASP VAL LYS LYS PHE VAL ALA ALA GLY THR CYS ALA PRO VAL LEU LEU ALA SER ASN PRO ALA PHE
ALA ALA PHE VAL GLU GLU ARG MET ASN GLY ASP GLY T73 G74 R75 A76 L88 S93 W96 Q103 D109 E110 G115 LEU THR LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.922	Depositor
Minimum map value	-0.284	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	624.0, 624.0, 624.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, FE2, DGD, 0UR, NEX, PHO, SQD, OEX, LMG, 8CT, 0IE, LHG, CHL, XAT, PL9, CLA, HEM

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	Z	0.18	0/486	0.28	0/664
1	z	0.17	0/486	0.28	0/664
2	E	0.42	0/546	0.54	1/745 (0.1%)
2	e	0.23	0/546	0.35	0/745
3	H	0.22	0/523	0.29	0/713
3	h	0.23	0/523	0.32	0/713
4	I	0.33	0/283	0.28	0/383
4	i	0.34	0/283	0.38	0/383
5	K	0.26	0/310	0.52	0/426
5	k	0.25	0/310	0.35	0/426
6	L	0.27	0/312	0.30	0/424
6	l	0.27	0/312	0.29	0/424
7	M	0.16	0/234	0.31	0/320
7	m	0.15	0/234	0.30	0/320
8	R	0.18	0/1749	0.41	2/2373 (0.1%)
8	r	0.18	0/1745	0.42	2/2369 (0.1%)
9	F	0.21	0/252	0.41	0/341
9	f	0.21	0/258	0.38	0/349
10	1	0.11	0/1658	0.30	0/2257
10	4	0.11	0/1652	0.30	0/2250
11	2	0.15	0/1763	0.33	0/2394
11	5	0.14	0/1764	0.29	0/2395
12	3	0.14	0/1657	0.36	0/2261
12	6	0.14	0/1722	0.40	1/2349 (0.0%)
12	7	0.19	0/1730	0.43	0/2359
12	9	0.12	0/1733	0.37	0/2363
12	p	0.19	0/1733	0.45	0/2363
12	u	0.13	0/1736	0.38	0/2367
13	S	0.25	0/1920	0.43	1/2621 (0.0%)
13	s	0.28	0/1920	0.45	1/2621 (0.0%)
14	X	0.14	0/227	0.22	0/308

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	x	0.14	0/227	0.22	0/308
15	V	0.13	0/179	0.38	0/245
15	v	0.13	0/179	0.36	0/245
16	T	0.30	0/244	0.36	0/329
16	t	0.31	0/244	0.35	0/329
17	8	0.19	0/1602	0.29	0/2182
17	G	0.11	0/1743	0.27	0/2371
17	N	0.14	0/1599	0.30	0/2178
17	Y	0.24	0/1743	0.31	0/2371
17	g	0.11	0/1743	0.26	0/2371
17	n	0.13	0/1592	0.29	0/2168
17	q	0.19	0/1602	0.29	0/2182
17	y	0.23	0/1743	0.29	0/2371
18	B	0.33	0/3866	0.37	1/5266 (0.0%)
18	b	0.27	0/3866	0.34	0/5266
19	A	0.33	0/2637	0.36	0/3595
19	a	0.41	0/2637	0.39	0/3595
20	C	0.30	0/3591	0.38	0/4895
20	c	0.30	0/3591	0.39	0/4895
21	D	0.33	0/2813	0.37	0/3832
21	d	0.35	0/2813	0.37	0/3832
22	W	0.24	0/308	0.51	0/417
22	w	0.23	0/308	0.51	0/417
All	All	0.25	0/71477	0.36	9/97350 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	77	GLY	N-CA-C	7.09	123.47	114.25
8	r	68	ASP	CA-C-N	-6.62	113.97	120.52
8	r	68	ASP	C-N-CA	-6.62	113.97	120.52
8	R	68	ASP	CA-C-N	-6.58	114.00	120.52
8	R	68	ASP	C-N-CA	-6.58	114.00	120.52
12	6	249	THR	CB-CA-C	-5.87	109.79	116.54
18	B	281	ALA	N-CA-C	-5.67	108.16	114.62
13	S	299	ILE	N-CA-C	-5.50	107.02	111.91
13	s	299	ILE	N-CA-C	-5.37	107.13	111.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	472	0	496	9	0
1	z	472	0	496	6	0
2	E	530	0	517	20	0
2	e	530	0	517	9	0
3	H	513	0	517	18	0
3	h	513	0	517	17	0
4	I	275	0	282	4	0
4	i	275	0	282	4	0
5	K	299	0	311	7	0
5	k	299	0	311	4	0
6	L	304	0	313	16	0
6	l	304	0	313	14	0
7	M	231	0	261	9	0
7	m	231	0	261	11	0
8	R	1711	0	1670	83	0
8	r	1707	0	1659	70	0
9	F	246	0	256	4	0
9	f	251	0	261	4	0
10	1	1609	0	1517	52	0
10	4	1603	0	1506	50	0
11	2	1710	0	1616	46	0
11	5	1711	0	1620	48	0
12	3	1606	0	1501	44	0
12	6	1670	0	1564	50	0
12	7	1677	0	1573	66	0
12	9	1680	0	1575	71	0
12	p	1680	0	1575	65	0
12	u	1683	0	1584	74	0
13	S	1867	0	1797	79	0
13	s	1867	0	1797	75	0
14	X	226	0	242	4	0
14	x	226	0	242	2	0
15	V	179	0	205	7	0
15	v	179	0	205	5	0
16	T	236	0	239	5	0
16	t	236	0	239	5	0
17	8	1554	0	1467	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1690	0	1593	57	0
17	N	1551	0	1458	64	0
17	Y	1690	0	1593	44	0
17	g	1690	0	1593	57	0
17	n	1545	0	1455	59	0
17	q	1554	0	1467	52	0
17	y	1690	0	1593	43	0
18	B	3737	0	3605	100	0
18	b	3737	0	3605	92	0
19	A	2558	0	2469	75	0
19	a	2558	0	2469	70	0
20	C	3472	0	3381	85	0
20	c	3472	0	3381	83	0
21	D	2719	0	2631	69	0
21	d	2719	0	2631	66	0
22	W	304	0	276	8	0
22	w	304	0	276	11	0
23	E	43	0	30	2	0
23	f	43	0	30	3	0
24	1	349	0	234	24	0
24	2	353	0	234	11	0
24	3	365	0	250	31	0
24	4	349	0	234	22	0
24	5	353	0	234	15	0
24	6	365	0	250	37	0
24	7	397	0	311	35	0
24	8	351	0	270	24	0
24	9	397	0	311	25	0
24	G	433	0	370	40	0
24	N	404	0	311	20	0
24	R	277	0	186	17	0
24	S	331	0	233	14	0
24	Y	486	0	411	26	0
24	g	433	0	370	28	0
24	n	404	0	311	21	0
24	p	397	0	311	37	0
24	q	404	0	311	23	0
24	r	277	0	186	19	0
24	s	331	0	233	14	0
24	u	397	0	311	21	0
24	y	433	0	370	26	0
25	1	268	0	204	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	305	0	258	10	0
25	3	256	0	186	6	0
25	4	268	0	204	23	0
25	5	305	0	258	11	0
25	6	256	0	186	7	0
25	7	321	0	280	27	0
25	8	310	0	267	12	0
25	9	324	0	284	16	0
25	A	280	0	271	12	0
25	B	980	0	1023	63	0
25	C	790	0	814	30	0
25	D	130	0	144	10	0
25	G	318	0	272	27	0
25	N	310	0	267	13	0
25	R	325	0	247	17	0
25	S	333	0	261	10	0
25	Y	321	0	278	8	0
25	a	280	0	271	13	0
25	b	980	0	1023	61	0
25	c	790	0	814	33	0
25	d	130	0	144	10	0
25	g	318	0	272	15	0
25	n	310	0	267	12	0
25	p	324	0	284	24	0
25	q	310	0	267	12	0
25	r	325	0	247	18	0
25	s	332	0	261	13	0
25	u	324	0	284	16	0
25	y	321	0	278	12	0
26	1	44	0	0	0	0
26	2	88	0	0	1	0
26	3	87	0	0	2	0
26	4	44	0	0	0	0
26	5	88	0	0	0	0
26	6	43	0	0	2	0
26	7	88	0	0	2	0
26	8	44	0	0	0	0
26	9	88	0	0	3	0
26	G	88	0	0	0	0
26	N	44	0	0	0	0
26	R	44	0	0	1	0
26	Y	88	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	g	88	0	0	0	0
26	n	44	0	0	0	0
26	p	88	0	0	2	0
26	q	44	0	0	0	0
26	r	44	0	0	1	0
26	u	88	0	0	1	0
26	y	88	0	0	2	0
27	R	44	0	56	16	0
27	r	44	0	56	8	0
28	1	44	0	56	22	0
28	2	44	0	56	9	0
28	3	44	0	56	22	0
28	4	44	0	56	21	0
28	5	44	0	56	10	0
28	6	44	0	56	21	0
28	7	44	0	56	32	0
28	9	44	0	56	6	0
28	G	44	0	56	32	0
28	N	44	0	56	7	0
28	R	44	0	56	6	0
28	S	44	0	56	24	0
28	g	44	0	56	15	0
28	n	44	0	56	7	0
28	p	44	0	56	27	0
28	r	88	0	112	15	0
28	s	44	0	56	21	0
28	u	44	0	56	9	0
28	y	44	0	56	4	0
29	1	52	0	0	0	0
29	2	52	0	0	1	0
29	3	52	0	0	0	0
29	4	52	0	0	1	0
29	5	52	0	0	0	0
29	6	52	0	0	1	0
29	7	52	0	0	0	0
29	8	52	0	0	1	0
29	9	52	0	0	1	0
29	G	52	0	0	1	0
29	N	52	0	0	0	0
29	Y	52	0	0	1	0
29	g	52	0	0	0	0
29	n	52	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	p	52	0	0	1	0
29	q	52	0	0	1	0
29	u	52	0	0	1	0
29	y	52	0	0	1	0
30	1	42	0	54	3	0
30	2	40	0	50	2	0
30	4	42	0	54	3	0
30	5	43	0	56	2	0
30	7	37	0	44	3	0
30	9	43	0	56	6	0
30	A	89	0	124	8	0
30	C	32	0	34	0	0
30	D	88	0	122	13	0
30	G	43	0	56	1	0
30	N	43	0	56	4	0
30	Y	43	0	56	0	0
30	a	89	0	124	7	0
30	c	32	0	34	0	0
30	d	88	0	122	11	0
30	g	43	0	56	2	0
30	n	43	0	56	4	0
30	p	43	0	56	3	0
30	y	43	0	56	2	0
31	A	40	0	0	0	0
31	B	40	0	0	0	0
31	C	120	0	0	1	0
31	D	40	0	0	0	0
31	S	80	0	0	0	0
31	T	40	0	0	0	0
31	V	40	0	0	1	0
31	X	40	0	0	0	0
31	a	40	0	0	0	0
31	b	40	0	0	0	0
31	c	120	0	0	1	0
31	d	40	0	0	0	0
31	s	80	0	0	0	0
31	t	40	0	0	0	0
31	v	40	0	0	1	0
31	x	40	0	0	0	0
32	A	45	0	54	2	0
32	B	54	0	78	4	0
32	D	44	0	52	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	a	45	0	54	4	0
32	b	54	0	78	5	0
32	d	44	0	52	1	0
33	B	41	0	52	5	0
33	C	42	0	54	6	0
33	D	94	0	128	8	0
33	W	30	0	30	2	0
33	d	94	0	128	8	0
33	i	48	0	66	3	0
33	m	41	0	52	6	0
33	w	36	0	42	6	0
34	A	10	0	0	0	0
34	a	10	0	0	0	0
35	A	64	0	74	4	0
35	D	64	0	74	6	0
35	a	64	0	74	4	0
35	d	64	0	74	6	0
36	A	4	0	1	0	0
36	a	4	0	1	0	0
37	C	105	0	126	7	0
37	c	105	0	126	8	0
38	D	1	0	0	0	0
38	d	1	0	0	0	0
39	D	55	0	80	2	0
39	d	55	0	80	2	0
All	All	95298	0	87326	2639	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 (2639) 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:S:58:TRP:HZ2	28:S:617:NEX:H183	1.14	1.10
12:u:158:LEU:HD23	28:u:304:NEX:H203	1.35	1.07
13:S:58:TRP:CZ2	28:S:617:NEX:H183	1.89	1.06
28:p:304:NEX:H31	24:p:310:CHL:HBA1	1.38	1.04
13:S:58:TRP:HE1	28:S:617:NEX:H192	1.19	1.03
28:g:304:NEX:H31	24:g:310:CHL:HBA1	1.41	1.01
28:4:303:NEX:H31	24:4:309:CHL:CBA	1.91	1.00
24:3:309:CHL:HBA2	28:3:318:NEX:H28	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:303:NEX:H362	25:4:307:CLA:C3B	1.91	1.00
13:s:58:TRP:HE1	28:s:401:NEX:H192	1.25	0.97
28:7:304:NEX:H362	25:7:308:CLA:C4B	1.97	0.94
28:G:304:NEX:H383	25:G:308:CLA:C1B	1.98	0.94
28:7:304:NEX:H383	25:7:308:CLA:C1B	1.98	0.94
28:7:304:NEX:H362	25:7:308:CLA:CHC	1.98	0.93
13:S:58:TRP:NE1	28:S:617:NEX:H192	1.81	0.93
28:p:304:NEX:C31	24:p:310:CHL:HBA1	1.98	0.93
28:6:303:NEX:H28	24:6:309:CHL:HBA2	1.52	0.92
28:7:304:NEX:C31	24:7:310:CHL:HBA1	1.98	0.92
13:S:59:PHE:HE2	28:S:617:NEX:O3	1.50	0.92
28:G:304:NEX:C15	24:G:312:CHL:CMB	2.50	0.89
28:p:304:NEX:H383	25:p:308:CLA:C1B	2.02	0.89
13:S:59:PHE:CE2	28:S:617:NEX:O3	2.24	0.89
8:R:67:PHE:HE2	27:R:615:XAT:H383	1.38	0.89
28:7:304:NEX:H31	24:7:310:CHL:HBA1	1.52	0.88
13:S:58:TRP:HZ2	28:S:617:NEX:C18	1.86	0.86
28:1:303:NEX:H383	25:1:307:CLA:C1B	2.05	0.86
28:g:304:NEX:C31	24:g:310:CHL:HBA1	2.05	0.86
13:S:59:PHE:CD2	28:S:617:NEX:H22	2.11	0.85
28:G:304:NEX:H362	25:G:308:CLA:CHC	2.07	0.85
19:a:296:ASN:HB3	20:c:389:LEU:HA	1.57	0.85
28:p:304:NEX:H362	25:p:308:CLA:C4B	2.06	0.85
8:r:48:MET:HE2	24:r:302:CHL:HHB	1.58	0.85
24:Y:308:CHL:HHB	8:r:172:LEU:HD13	1.59	0.85
28:7:304:NEX:H403	24:7:310:CHL:CBA	2.06	0.85
8:R:67:PHE:CE2	27:R:615:XAT:H242	2.11	0.85
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.58	0.84
25:r:305:CLA:C1B	28:r:317:NEX:H383	2.09	0.83
17:N:101:TYR:HB3	17:N:107:LEU:HD23	1.58	0.83
28:7:304:NEX:H403	24:7:310:CHL:HBA1	1.59	0.83
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.59	0.83
12:3:236:ASP:HB3	12:3:240:ASN:HB2	1.60	0.82
28:4:303:NEX:H383	25:4:307:CLA:C1B	2.09	0.82
25:R:604:CLA:C1B	28:R:616:NEX:H383	2.09	0.82
8:R:172:LEU:HD13	24:y:309:CHL:HHB	1.59	0.82
28:S:617:NEX:H31	24:8:308:CHL:HBA2	1.59	0.82
20:C:398:VAL:HG22	20:C:401:GLU:HB2	1.62	0.82
18:B:46:ASP:H	18:B:58:GLN:HE22	1.27	0.81
28:1:303:NEX:H31	24:1:309:CHL:CBA	2.10	0.81
24:3:309:CHL:HAA1	28:3:318:NEX:O24	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:LYS:HG2	8:R:80:GLN:HE22	1.46	0.81
28:1:303:NEX:C15	24:1:311:CHL:HMB2	2.11	0.81
11:5:185:VAL:HG21	25:5:317:CLA:HAC2	1.62	0.80
24:3:309:CHL:CAA	28:3:318:NEX:O24	2.30	0.80
11:2:185:VAL:HG21	25:2:317:CLA:HAC2	1.62	0.80
28:G:304:NEX:H222	25:G:308:CLA:C1C	2.11	0.80
13:S:211:TYR:HB3	13:S:215:ILE:HB	1.64	0.80
13:s:211:TYR:HB3	13:s:215:ILE:HB	1.63	0.79
18:b:46:ASP:H	18:b:58:GLN:HE22	1.27	0.79
20:c:398:VAL:HG22	20:c:401:GLU:HB2	1.66	0.78
24:3:309:CHL:CBA	28:3:318:NEX:H28	2.14	0.78
17:n:101:TYR:HB3	17:n:107:LEU:HD23	1.66	0.78
12:7:168:PRO:HG2	24:7:312:CHL:HBB2	1.66	0.77
28:4:303:NEX:H222	25:4:307:CLA:C4B	2.14	0.77
18:B:480:ALA:H	21:D:139:ARG:HH12	1.32	0.77
28:4:303:NEX:H362	25:4:307:CLA:C4B	2.15	0.76
25:r:305:CLA:C2B	28:r:317:NEX:H383	2.15	0.76
17:8:137:LEU:HG	24:8:309:CHL:HBB1	1.67	0.76
28:6:303:NEX:C28	24:6:309:CHL:HAA1	2.15	0.76
28:1:303:NEX:C15	24:1:311:CHL:CMB	2.64	0.76
17:g:137:LEU:HG	24:g:312:CHL:HBB1	1.67	0.76
13:s:58:TRP:NE1	28:s:401:NEX:H192	2.00	0.76
8:R:48:MET:HE2	24:R:601:CHL:HHB	1.67	0.76
8:r:87:ASP:HB2	8:r:90:ALA:HB3	1.68	0.76
28:4:303:NEX:H362	25:4:307:CLA:CAB	2.14	0.76
12:p:230:TRP:HE1	24:p:318:CHL:HMC	1.51	0.76
6:L:12:GLU:HA	7:M:29:THR:HG21	1.68	0.75
12:u:158:LEU:HD23	28:u:304:NEX:C20	2.15	0.75
3:h:57:TYR:HD2	25:b:602:CLA:H2	1.50	0.75
28:S:617:NEX:H383	25:8:306:CLA:C2B	2.17	0.75
12:p:217:VAL:HG21	25:p:317:CLA:HAC2	1.69	0.75
8:R:69:PRO:HG2	27:R:615:XAT:H221	1.69	0.74
13:S:59:PHE:CE2	28:S:617:NEX:H22	2.21	0.74
12:7:217:VAL:HG21	25:7:317:CLA:HAC2	1.68	0.74
17:8:185:VAL:HG21	25:8:314:CLA:HAC2	1.69	0.74
18:b:480:ALA:H	21:d:139:ARG:HH12	1.36	0.74
15:V:295:LEU:HA	15:V:298:VAL:HG12	1.69	0.74
24:q:310:CHL:HMA3	28:s:401:NEX:H30	1.69	0.74
12:p:168:PRO:HB2	24:p:312:CHL:HBB2	1.71	0.73
25:a:604:CLA:HHC	25:a:604:CLA:HBB1	1.71	0.73
28:1:303:NEX:H362	25:1:307:CLA:C4B	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:131:TRP:HZ2	20:C:437:ARG:HG2	1.53	0.73
12:u:242:ILE:HD13	25:u:317:CLA:HMD3	1.69	0.73
12:3:103:GLU:HA	12:3:116:PRO:HB2	1.70	0.73
13:S:59:PHE:CE2	28:S:617:NEX:C2	2.72	0.73
6:l:12:GLU:HA	7:m:29:THR:HG21	1.70	0.73
24:4:311:CHL:HHC	24:4:311:CHL:HBB1	1.71	0.73
21:d:161:PRO:HB3	21:d:170:ALA:HB2	1.69	0.73
21:D:161:PRO:HB3	21:D:170:ALA:HB2	1.70	0.73
15:v:295:LEU:HA	15:v:298:VAL:HG12	1.71	0.72
17:N:171:LYS:NZ	30:N:318:LHG:O4	2.21	0.72
28:7:304:NEX:C36	25:7:308:CLA:CHC	2.67	0.72
3:H:57:TYR:HD2	25:B:602:CLA:H2	1.53	0.72
12:9:217:VAL:HG11	25:9:316:CLA:HAC2	1.69	0.72
12:7:230:TRP:HE1	24:7:318:CHL:HMC	1.54	0.72
28:p:304:NEX:H362	25:p:308:CLA:CHC	2.19	0.72
17:q:137:LEU:HG	24:q:310:CHL:HBB1	1.71	0.72
19:A:296:ASN:HB3	20:C:389:LEU:HA	1.70	0.72
19:a:131:TRP:HZ2	20:c:437:ARG:HG2	1.53	0.72
25:p:315:CLA:H41	25:p:315:CLA:H92	1.71	0.71
18:b:392:ILE:HD11	18:b:418:LYS:HG3	1.72	0.71
12:7:40:ARG:NH2	12:7:56:LEU:O	2.23	0.71
12:7:200:LYS:O	12:7:204:ASN:ND2	2.23	0.71
17:N:52:LEU:O	17:N:56:HIS:ND1	2.23	0.71
17:g:131:ARG:NH2	24:g:313:CHL:O1D	2.23	0.71
18:b:119:ASP:OD1	18:b:124:ARG:NH2	2.24	0.71
20:c:395:VAL:HG11	20:c:404:ALA:H	1.54	0.71
17:n:171:LYS:NZ	30:n:318:LHG:O4	2.22	0.71
24:1:311:CHL:HHC	24:1:311:CHL:HBB1	1.72	0.71
25:7:315:CLA:H41	25:7:315:CLA:H92	1.71	0.71
20:C:221:ILE:O	20:C:225:HIS:ND1	2.24	0.71
12:p:40:ARG:NH2	12:p:56:LEU:O	2.24	0.71
20:c:221:ILE:O	20:c:225:HIS:ND1	2.24	0.71
17:N:126:LEU:HB2	28:N:303:NEX:H203	1.72	0.71
19:A:57:PRO:HB2	19:A:66:PRO:HB2	1.73	0.71
33:i:101:LMG:HC71	20:c:204:SER:HB2	1.71	0.71
6:l:12:GLU:OE2	18:b:3:LEU:N	2.24	0.71
17:n:126:LEU:HB2	28:n:303:NEX:H203	1.73	0.70
25:A:604:CLA:HHC	25:A:604:CLA:HBB1	1.73	0.70
17:q:168:LYS:O	17:q:172:ASN:ND2	2.23	0.70
19:a:27:ARG:NH1	21:d:254:SER:O	2.24	0.70
20:c:449:ARG:NH2	21:d:242:GLU:O	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:119:ASP:OD1	18:B:124:ARG:NH2	2.24	0.70
28:4:303:NEX:C31	24:4:309:CHL:CBA	2.70	0.70
12:p:200:LYS:O	12:p:204:ASN:ND2	2.23	0.70
12:7:117:VAL:HG21	12:7:120:SER:HB2	1.74	0.70
12:9:74:ASP:H	12:9:77:MET:HE2	1.57	0.70
10:4:10:LEU:HG	10:4:20:VAL:HG11	1.72	0.70
28:5:304:NEX:H163	17:n:153:MET:HG2	1.73	0.70
24:q:304:CHL:HHC	24:q:304:CHL:HBB1	1.74	0.70
28:2:304:NEX:C17	17:N:152:PRO:HB2	2.22	0.70
17:8:168:LYS:O	17:8:172:ASN:ND2	2.24	0.69
28:p:304:NEX:H403	24:p:310:CHL:CBA	2.22	0.69
17:y:57:ALA:HB1	17:y:173:GLY:HA3	1.73	0.69
19:a:57:PRO:HB2	19:a:66:PRO:HB2	1.74	0.69
28:G:304:NEX:H362	25:G:308:CLA:C4B	2.22	0.69
28:7:304:NEX:H383	25:7:308:CLA:CHB	2.21	0.69
28:6:303:NEX:H28	24:6:309:CHL:CBA	2.23	0.69
13:S:120:ARG:HD3	24:S:602:CHL:HED1	1.75	0.69
28:G:304:NEX:C22	25:G:308:CLA:C1C	2.70	0.69
28:6:303:NEX:O24	24:6:309:CHL:HAA1	1.93	0.69
28:G:304:NEX:C36	25:G:308:CLA:CHC	2.70	0.69
18:B:392:ILE:HD11	18:B:418:LYS:HG3	1.74	0.69
13:s:59:PHE:CD2	28:s:401:NEX:H183	2.28	0.69
28:G:304:NEX:H222	25:G:308:CLA:CHC	2.23	0.69
18:B:276:ASP:OD1	18:B:276:ASP:N	2.26	0.69
24:R:605:CHL:CBB	27:R:615:XAT:H162	2.22	0.69
21:D:192:THR:HG23	25:D:404:CLA:HBC2	1.74	0.69
13:S:58:TRP:CZ2	28:S:617:NEX:C18	2.68	0.69
9:f:20:VAL:HG23	9:f:21:HIS:HD1	1.58	0.69
19:a:143:ILE:HD12	21:d:252:PHE:CE2	2.28	0.69
8:R:261:LEU:HB3	11:2:106:GLU:HB2	1.75	0.68
19:A:143:ILE:HD12	21:D:252:PHE:CE2	2.28	0.68
24:8:304:CHL:HHC	24:8:304:CHL:HBB1	1.75	0.68
19:A:27:ARG:NH1	21:D:254:SER:O	2.25	0.68
21:d:192:THR:HG23	25:d:404:CLA:HBC2	1.74	0.68
13:S:200:ASN:OD1	13:S:203:ARG:NH2	2.26	0.68
17:G:131:ARG:NH2	24:G:313:CHL:O1D	2.26	0.68
12:6:217:VAL:HG11	25:6:316:CLA:HAC2	1.75	0.68
17:Y:57:ALA:HB1	17:Y:173:GLY:HA3	1.73	0.68
12:3:217:VAL:HG11	25:3:316:CLA:HAC2	1.74	0.68
20:C:449:ARG:NH2	21:D:242:GLU:O	2.27	0.68
11:5:8:ARG:NH2	11:5:24:LEU:O	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:200:ASN:OD1	13:s:203:ARG:NH2	2.26	0.68
6:l:11:VAL:HG21	7:m:25:LEU:HD22	1.76	0.68
10:4:11:TRP:HB3	10:4:32:TYR:HB3	1.74	0.68
20:c:27:ASN:ND2	25:c:610:CLA:O1A	2.27	0.68
28:g:304:NEX:H31	24:g:310:CHL:CBA	2.20	0.67
20:C:27:ASN:ND2	25:C:610:CLA:O1A	2.26	0.67
6:L:11:VAL:HG21	7:M:25:LEU:HD22	1.75	0.67
17:n:52:LEU:O	17:n:56:HIS:ND1	2.24	0.67
5:K:7:LYS:N	20:C:61:ALA:O	2.28	0.67
28:p:304:NEX:H383	25:p:308:CLA:CHB	2.23	0.67
28:1:303:NEX:H362	25:1:307:CLA:C3B	2.24	0.67
24:3:309:CHL:HAA1	28:3:318:NEX:C28	2.24	0.67
12:u:74:ASP:H	12:u:77:MET:HE2	1.58	0.67
28:6:303:NEX:O24	24:6:309:CHL:CAA	2.43	0.67
12:9:236:ASP:O	12:9:239:ASN:ND2	2.28	0.67
12:u:89:SER:HB2	12:u:205:GLY:HA3	1.77	0.67
12:6:103:GLU:HA	12:6:116:PRO:HB2	1.76	0.67
11:2:8:ARG:NH2	11:2:24:LEU:O	2.27	0.67
12:9:89:SER:HB2	12:9:205:GLY:HA3	1.77	0.67
17:N:125:GLY:HA2	24:N:312:CHL:HAB	1.77	0.67
28:G:304:NEX:H383	25:G:308:CLA:C2B	2.24	0.67
12:p:229:ASN:ND2	25:p:317:CLA:O1D	2.28	0.67
28:p:304:NEX:H403	24:p:310:CHL:HBA1	1.76	0.67
18:b:130:LYS:HB2	8:r:83:ILE:HD12	1.76	0.67
20:C:216:ASP:OD1	20:C:350:ARG:NH1	2.28	0.66
17:g:189:GLN:NE2	17:g:213:TYR:O	2.27	0.66
25:b:606:CLA:H11	25:b:610:CLA:H13	1.77	0.66
18:B:152:GLY:O	18:B:153:PHE:C	2.37	0.66
12:9:200:LYS:NZ	25:9:315:CLA:O1A	2.28	0.66
13:s:253:LYS:O	13:s:257:ASN:ND2	2.29	0.66
12:9:203:LYS:NZ	30:9:318:LHG:O4	2.28	0.66
10:1:36:SER:O	12:3:80:GLN:NE2	2.28	0.66
17:N:45:THR:O	17:N:49:ASN:ND2	2.27	0.66
10:1:11:TRP:HB3	10:1:32:TYR:HB3	1.77	0.66
3:h:58:ASN:ND2	3:h:60:ASP:OD2	2.29	0.66
17:n:51:GLU:HA	17:n:144:LEU:HD11	1.78	0.66
17:g:101:TYR:HH	28:g:304:NEX:H1	1.43	0.66
28:S:617:NEX:H30	24:8:309:CHL:HMA3	1.78	0.66
5:k:7:LYS:N	20:c:61:ALA:O	2.29	0.66
17:G:137:LEU:HG	24:G:312:CHL:HBB1	1.77	0.66
20:c:216:ASP:OD1	20:c:350:ARG:NH1	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:d:139:ARG:HE	21:d:141:TYR:HE2	1.44	0.65
13:s:120:ARG:HD3	24:s:403:CHL:HED1	1.77	0.65
12:7:229:ASN:ND2	25:7:317:CLA:O1D	2.29	0.65
28:2:304:NEX:H172	17:N:152:PRO:HB2	1.79	0.65
25:R:610:CLA:H2A	25:R:610:CLA:HED3	1.78	0.65
24:3:309:CHL:HAA1	28:3:318:NEX:C27	2.26	0.65
13:S:253:LYS:O	13:S:257:ASN:ND2	2.29	0.65
12:9:45:GLY:HA3	24:9:304:CHL:HBB1	1.79	0.65
8:R:186:VAL:HG23	24:R:608:CHL:HBB2	1.78	0.65
20:C:204:SER:HB2	33:C:618:LMG:HC71	1.78	0.65
28:6:303:NEX:C27	24:6:309:CHL:HAA1	2.27	0.65
28:g:304:NEX:H362	25:g:308:CLA:C4B	2.27	0.65
17:y:198:TRP:HE1	24:y:318:CHL:HMC	1.61	0.65
24:Y:309:CHL:HHC	24:Y:309:CHL:HBB1	1.79	0.65
28:4:303:NEX:H222	25:4:307:CLA:NB	2.12	0.65
21:D:129:GLN:NE2	35:D:403:PHO:OBD	2.30	0.65
19:a:334:ARG:HH22	21:d:320:LEU:HD12	1.62	0.65
13:S:86:ASP:N	13:S:86:ASP:OD1	2.30	0.64
25:r:304:CLA:HBC1	24:r:309:CHL:HBC2	1.79	0.64
12:7:133:TYR:HE1	28:7:304:NEX:H1	1.40	0.64
25:R:603:CLA:HBC1	24:R:608:CHL:HBC2	1.79	0.64
12:p:203:LYS:NZ	30:p:319:LHG:O4	2.31	0.64
17:8:45:THR:O	17:8:49:ASN:ND2	2.30	0.64
21:d:129:GLN:NE2	35:d:403:PHO:OBD	2.30	0.64
12:6:200:LYS:O	12:6:204:ASN:ND2	2.26	0.64
12:9:40:ARG:NH2	12:9:56:LEU:O	2.31	0.64
24:R:602:CHL:CBB	27:R:615:XAT:H32	2.27	0.64
13:S:283:TRP:HE1	24:S:613:CHL:HMC	1.62	0.64
13:s:283:TRP:HE1	24:s:414:CHL:HMC	1.62	0.64
13:s:86:ASP:OD1	13:s:86:ASP:N	2.30	0.64
28:p:304:NEX:H403	24:p:310:CHL:CGA	2.28	0.64
24:1:309:CHL:HHC	24:1:309:CHL:HBB1	1.80	0.64
17:G:94:PHE:HZ	12:9:243:PHE:HB3	1.62	0.64
12:6:128:ASP:O	12:6:143:GLN:NE2	2.30	0.64
20:c:390:GLY:HA3	20:c:408:VAL:HG22	1.79	0.64
28:7:304:NEX:H241	25:7:308:CLA:H2	1.79	0.64
25:B:606:CLA:H11	25:B:610:CLA:H13	1.80	0.63
28:4:303:NEX:C31	24:4:309:CHL:H3A	2.28	0.63
28:g:304:NEX:H383	25:g:308:CLA:C1B	2.28	0.63
8:r:82:ASP:N	8:r:82:ASP:OD1	2.30	0.63
28:p:304:NEX:C40	24:p:310:CHL:O2A	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:173:VAL:HG12	13:s:175:TRP:H	1.64	0.63
8:R:83:ILE:HD12	18:B:130:LYS:HB2	1.80	0.63
12:7:203:LYS:NZ	30:7:319:LHG:O4	2.31	0.63
12:3:128:ASP:O	12:3:143:GLN:NE2	2.31	0.63
24:3:309:CHL:HAA1	28:3:318:NEX:C26	2.27	0.63
17:q:45:THR:O	17:q:49:ASN:ND2	2.30	0.63
28:4:303:NEX:C36	25:4:307:CLA:HAB	2.28	0.63
24:n:308:CHL:HAA2	25:r:313:CLA:HBA2	1.79	0.63
6:L:12:GLU:OE2	18:B:3:LEU:N	2.32	0.63
8:R:160:GLU:OE2	8:R:164:GLN:NE2	2.31	0.63
17:g:101:TYR:HB3	17:g:107:LEU:HG	1.80	0.63
17:Y:198:TRP:HE1	24:Y:317:CHL:HMC	1.62	0.63
17:y:85:VAL:HG23	17:y:88:LYS:HB2	1.80	0.63
24:y:310:CHL:HBB1	24:y:310:CHL:HHC	1.80	0.63
11:2:57:ALA:HB1	11:2:173:GLY:HA3	1.79	0.63
13:S:98:LEU:HD22	13:S:120:ARG:HG3	1.81	0.63
17:Y:10:LEU:HD23	17:Y:16:SER:HB2	1.79	0.63
11:5:57:ALA:HB1	11:5:173:GLY:HA3	1.79	0.63
12:u:250:ARG:H	12:u:250:ARG:HE	1.47	0.63
17:n:125:GLY:HA2	24:n:312:CHL:HAB	1.79	0.63
25:B:609:CLA:H202	25:B:612:CLA:H18	1.80	0.63
3:H:58:ASN:ND2	3:H:60:ASP:OD2	2.32	0.62
20:C:395:VAL:HG11	20:C:403:ASN:HA	1.81	0.62
17:q:101:TYR:HB2	17:q:108:VAL:HG22	1.81	0.62
20:c:33:LEU:HA	20:c:127:THR:HG22	1.80	0.62
8:r:163:LEU:HB2	24:r:307:CHL:HMD1	1.79	0.62
17:G:128:GLU:OE1	17:G:131:ARG:NH1	2.32	0.62
28:G:304:NEX:C20	24:G:312:CHL:HMB1	2.28	0.62
13:S:124:LEU:HD13	13:S:229:LEU:HB3	1.81	0.62
20:C:33:LEU:HA	20:C:127:THR:HG22	1.80	0.62
10:4:125:GLY:HA2	24:4:312:CHL:HAB	1.82	0.62
28:5:304:NEX:H21	17:n:153:MET:HA	1.82	0.62
18:b:467:ILE:HD13	21:d:126:MET:HE1	1.80	0.62
32:d:409:SQD:H291	33:d:411:LMG:H192	1.80	0.62
12:3:200:LYS:O	12:3:204:ASN:ND2	2.26	0.62
19:A:45:THR:HG23	25:A:604:CLA:H201	1.81	0.62
19:A:334:ARG:HH22	21:D:320:LEU:HD12	1.63	0.62
25:q:306:CLA:NB	28:s:401:NEX:H242	2.15	0.62
19:a:45:THR:HG23	25:a:604:CLA:H201	1.81	0.62
8:r:135:ARG:NE	8:r:232:GLU:OE2	2.25	0.62
24:9:309:CHL:HBC2	24:9:310:CHL:HHD	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:136:PRO:HG3	13:s:58:TRP:CD2	2.35	0.62
8:R:64:ASP:O	8:R:65:ARG:NH1	2.31	0.62
28:p:304:NEX:H31	24:p:310:CHL:CBA	2.23	0.62
17:Y:21:PRO:HG2	17:Y:35:ASP:HB3	1.81	0.62
12:p:236:ASP:O	12:p:239:ASN:ND2	2.31	0.62
17:G:171:LYS:NZ	30:G:319:LHG:O4	2.32	0.62
17:G:211:PHE:HB3	17:N:94:PHE:HZ	1.65	0.62
17:N:126:LEU:HB2	28:N:303:NEX:C20	2.30	0.62
11:5:106:GLU:HB2	8:r:261:LEU:HB3	1.82	0.62
14:X:84:VAL:HG21	24:G:318:CHL:HMB2	1.81	0.62
17:Y:71:GLU:HA	17:Y:84:ALA:HB1	1.81	0.62
21:D:139:ARG:HE	21:D:141:TYR:HE2	1.45	0.62
17:Y:85:VAL:HG23	17:Y:88:LYS:HB2	1.80	0.61
2:e:98:ARG:NH2	3:h:59:SER:OG	2.33	0.61
12:7:248:ILE:O	12:7:252:ALA:N	2.33	0.61
18:B:467:ILE:HD13	21:D:126:MET:HE1	1.81	0.61
21:d:186:GLN:HB2	25:d:404:CLA:HBC1	1.81	0.61
10:1:131:ARG:NH2	24:1:312:CHL:O1D	2.30	0.61
25:A:605:CLA:HAB	25:D:404:CLA:H51	1.82	0.61
10:4:131:ARG:NH2	24:4:312:CHL:O1D	2.31	0.61
10:4:158:ASP:HB3	10:4:161:THR:HG22	1.82	0.61
28:G:304:NEX:C15	24:G:312:CHL:HMB1	2.29	0.61
17:N:128:GLU:OE1	17:N:131:ARG:NH2	2.33	0.61
13:s:180:ASN:ND2	24:s:406:CHL:OBD	2.34	0.61
25:r:305:CLA:CHC	28:r:317:NEX:H222	2.30	0.61
10:1:130:TYR:OH	28:1:303:NEX:C19	2.48	0.61
17:G:118:TRP:HZ2	24:9:317:CHL:HBD	1.65	0.61
17:Y:19:ALA:HB2	17:8:132:CYS:HB3	1.82	0.61
13:s:98:LEU:HD22	13:s:120:ARG:HG3	1.81	0.61
21:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.81	0.61
18:b:372:ASP:OD1	18:b:373:ASP:N	2.32	0.61
8:R:135:ARG:NE	8:R:232:GLU:OE2	2.26	0.61
11:2:51:GLU:HA	11:2:144:LEU:HD21	1.82	0.61
12:9:118:TRP:HE1	12:9:219:ALA:HB2	1.66	0.61
20:C:390:GLY:HA3	20:C:408:VAL:HG22	1.82	0.61
30:D:408:LHG:HC41	30:D:408:LHG:HC11	1.81	0.61
10:4:100:ASP:OD2	10:4:109:HIS:ND1	2.32	0.61
13:s:59:PHE:CD2	28:s:401:NEX:C18	2.83	0.61
13:S:58:TRP:CD1	28:S:617:NEX:H192	2.35	0.61
28:p:304:NEX:H241	25:p:308:CLA:O2A	2.00	0.61
20:c:444:GLU:OE2	20:c:445:LYS:NZ	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:r:214:PRO:C	28:r:301:NEX:O3	2.43	0.61
13:S:173:VAL:HG12	13:S:175:TRP:H	1.65	0.61
11:5:9:GLU:HB3	24:5:305:CHL:HBC1	1.81	0.61
11:5:112:SER:N	24:5:309:CHL:OMC	2.34	0.61
17:g:128:GLU:OE1	17:g:131:ARG:NH1	2.33	0.61
10:1:125:GLY:HA2	24:1:312:CHL:HAB	1.81	0.61
10:1:158:ASP:HB3	10:1:161:THR:HG22	1.82	0.61
13:S:240:LEU:HD23	25:S:609:CLA:H11	1.82	0.60
17:G:201:HIS:CG	25:G:317:CLA:HAA2	2.36	0.60
19:A:63:ILE:HD12	20:C:323:THR:HB	1.82	0.60
25:9:316:CLA:HAB	30:9:318:LHG:H332	1.83	0.60
17:N:85:VAL:HG23	17:N:88:LYS:HB2	1.83	0.60
12:u:61:PRO:HB2	12:u:202:ILE:HD12	1.83	0.60
17:y:137:LEU:HG	24:y:312:CHL:HBB1	1.83	0.60
13:s:58:TRP:C	13:s:60:GLY:H	2.09	0.60
28:7:304:NEX:C40	24:7:310:CHL:HBA1	2.29	0.60
11:2:1:VAL:HG12	11:2:3:TRP:H	1.67	0.60
17:g:51:GLU:HA	17:g:144:LEU:HD21	1.84	0.60
17:n:185:VAL:HG21	25:n:316:CLA:HAC2	1.82	0.60
17:y:21:PRO:HG2	17:y:35:ASP:HB3	1.82	0.60
17:y:71:GLU:HA	17:y:84:ALA:HB1	1.82	0.60
32:a:609:SQD:H311	25:c:608:CLA:H92	1.82	0.60
21:d:79:SER:HA	21:d:172:SER:HB3	1.81	0.60
11:2:168:LYS:HD3	25:2:316:CLA:HAA2	1.82	0.60
24:4:309:CHL:HHC	24:4:309:CHL:HBB1	1.84	0.60
17:g:201:HIS:CG	25:g:317:CLA:HAA2	2.36	0.60
25:b:602:CLA:H42	33:d:401:LMG:H112	1.83	0.60
11:2:9:GLU:HB3	24:2:305:CHL:HBC1	1.82	0.60
17:q:123:LEU:HD22	28:s:401:NEX:C14	2.32	0.60
19:a:63:ILE:HD12	20:c:323:THR:HB	1.82	0.60
11:5:1:VAL:HG12	11:5:3:TRP:H	1.66	0.60
25:y:307:CLA:HBB1	24:y:313:CHL:H161	1.84	0.60
21:d:32:TRP:CD1	33:d:411:LMG:H111	2.37	0.60
28:7:304:NEX:H403	24:7:310:CHL:CGA	2.31	0.60
17:g:171:LYS:NZ	30:g:319:LHG:O4	2.33	0.60
17:y:221:GLN:NE2	17:y:223:PHE:OXT	2.35	0.60
28:G:304:NEX:H362	25:G:308:CLA:HAB	1.83	0.60
28:G:304:NEX:H222	25:G:308:CLA:NC	2.17	0.60
21:D:79:SER:HA	21:D:172:SER:HB3	1.83	0.60
28:5:304:NEX:C17	17:n:152:PRO:HB2	2.32	0.60
12:u:40:ARG:NH2	12:u:56:LEU:O	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:n:42:ASP:HB3	17:n:45:THR:HG22	1.84	0.60
10:4:58:ARG:NH1	24:4:311:CHL:OBD	2.32	0.59
17:y:19:ALA:HB2	17:q:132:CYS:HB3	1.83	0.59
12:3:44:LEU:HB3	12:3:47:TYR:HB2	1.84	0.59
11:5:168:LYS:HD3	25:5:316:CLA:HAA2	1.83	0.59
12:7:233:HIS:CG	25:7:317:CLA:HAA2	2.37	0.59
12:3:89:SER:HB3	12:3:205:GLY:HA3	1.84	0.59
25:3:307:CLA:HBA2	28:3:318:NEX:H241	1.84	0.59
17:N:42:ASP:HB3	17:N:45:THR:HG22	1.84	0.59
11:5:69:THR:HG21	25:5:308:CLA:HAC2	1.84	0.59
17:n:85:VAL:HG23	17:n:88:LYS:HB2	1.84	0.59
8:R:65:ARG:HB2	24:R:602:CHL:HMD1	1.84	0.59
8:R:87:ASP:HB2	8:R:90:ALA:HB3	1.84	0.59
17:G:101:TYR:HB3	17:G:107:LEU:HG	1.83	0.59
3:h:73:LEU:HD23	18:b:195:PRO:HD3	1.85	0.59
17:n:128:GLU:OE1	17:n:131:ARG:NH2	2.35	0.59
11:2:69:THR:HG21	25:2:308:CLA:HAC2	1.84	0.59
17:Y:221:GLN:NE2	17:Y:223:PHE:OXT	2.36	0.59
10:1:168:LYS:HD3	25:1:315:CLA:HAA2	1.85	0.59
21:D:189:HIS:HA	21:D:294:ARG:HD3	1.85	0.59
5:k:25:ILE:HD12	15:v:289:VAL:HG11	1.83	0.59
11:5:51:GLU:HA	11:5:144:LEU:HD21	1.85	0.59
12:6:236:ASP:HB3	12:6:240:ASN:HB2	1.84	0.59
12:u:157:SER:HB3	24:u:313:CHL:HAB	1.84	0.59
12:p:42:LEU:HD22	12:p:52:VAL:HG11	1.83	0.59
10:1:58:ARG:NH1	24:1:311:CHL:OBD	2.32	0.59
28:4:303:NEX:H383	25:4:307:CLA:CHB	2.32	0.59
8:r:213:ASP:OD1	26:r:315:0IE:O42	2.20	0.59
17:n:45:THR:O	17:n:49:ASN:ND2	2.27	0.59
8:r:65:ARG:HB2	24:r:303:CHL:HMD1	1.84	0.59
24:Y:312:CHL:HBB1	24:7:305:CHL:H52	1.85	0.59
12:7:41:ALA:HB1	24:7:305:CHL:HBC1	1.85	0.59
28:7:304:NEX:H31	24:7:310:CHL:CBA	2.27	0.59
19:A:267:ASN:ND2	21:D:232:PHE:O	2.36	0.59
12:p:183:ASP:OD1	29:p:301:0UR:O40	2.20	0.59
17:q:201:HIS:CG	25:q:315:CLA:HAA2	2.38	0.59
12:7:163:ARG:NH2	24:7:313:CHL:O1D	2.36	0.59
24:3:309:CHL:HBC2	24:3:310:CHL:HHD	1.85	0.58
24:3:311:CHL:HBB1	24:3:311:CHL:HHC	1.85	0.58
17:N:185:VAL:HG21	25:N:316:CLA:HAC2	1.83	0.58
17:g:88:LYS:HD3	24:g:311:CHL:HED2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:q:306:CLA:C4B	28:s:401:NEX:H242	2.33	0.58
10:1:185:VAL:HG21	25:1:316:CLA:HAC2	1.85	0.58
12:9:157:SER:HB3	24:9:312:CHL:HAB	1.85	0.58
10:4:185:VAL:HG21	25:4:316:CLA:HAC2	1.85	0.58
24:6:311:CHL:HHC	24:6:311:CHL:HBB1	1.85	0.58
14:x:84:VAL:HG21	24:g:318:CHL:HMB2	1.85	0.58
24:u:310:CHL:HHC	24:u:310:CHL:HBB1	1.86	0.58
24:y:313:CHL:HBB1	24:p:305:CHL:H52	1.85	0.58
20:c:395:VAL:HG23	20:c:407:PHE:H	1.68	0.58
21:d:262:SER:N	30:d:407:LHG:O5	2.35	0.58
8:R:224:LYS:NZ	11:2:151:ASP:O	2.35	0.58
11:2:112:SER:N	24:2:309:CHL:OMC	2.35	0.58
17:8:201:HIS:CG	25:8:314:CLA:HAA2	2.38	0.58
21:D:262:SER:N	30:D:407:LHG:O5	2.35	0.58
3:H:73:LEU:HD23	18:B:195:PRO:HD3	1.85	0.58
17:Y:137:LEU:HG	24:Y:311:CHL:HBB1	1.84	0.58
25:Y:306:CLA:HBB1	24:Y:312:CHL:H161	1.84	0.58
17:y:128:GLU:HA	17:y:131:ARG:HG2	1.86	0.58
8:r:73:SER:HB2	24:r:303:CHL:HAA2	1.86	0.58
10:1:2:GLU:O	10:1:9:ALA:N	2.36	0.58
17:n:101:TYR:HB2	17:n:108:VAL:HG12	1.85	0.58
12:p:52:VAL:HG12	12:p:65:GLY:HA3	1.85	0.58
8:r:86:LEU:HG	8:r:88:GLN:HG2	1.86	0.58
8:r:135:ARG:HD3	25:r:310:CLA:C4C	2.33	0.58
17:G:104:ASN:ND2	17:G:106:SER:OG	2.36	0.58
20:C:444:GLU:OE2	20:C:445:LYS:NZ	2.32	0.58
8:r:64:ASP:O	8:r:65:ARG:NH1	2.35	0.58
12:7:200:LYS:HD3	25:7:316:CLA:HAA2	1.86	0.58
8:R:69:PRO:HG2	27:R:615:XAT:C22	2.33	0.58
19:A:76:ASN:OD1	19:A:76:ASN:N	2.34	0.58
15:v:282:GLN:HG2	15:v:283:LEU:H	1.68	0.58
20:c:390:GLY:HA2	20:c:396:GLY:HA3	1.86	0.58
5:K:25:ILE:HD12	15:V:289:VAL:HG11	1.84	0.58
25:B:614:CLA:H42	32:B:618:SQD:H122	1.86	0.58
19:a:163:ILE:HD11	37:c:619:DGD:HA21	1.84	0.58
24:r:303:CHL:CBB	27:r:316:XAT:H32	2.34	0.58
10:1:168:LYS:O	10:1:172:ASN:ND2	2.25	0.58
12:9:90:ARG:NE	12:9:201:GLU:OE2	2.29	0.58
18:B:15:ASP:HB3	18:B:18:ARG:HB2	1.86	0.58
19:A:190:HIS:ND1	19:A:298:ASN:OD1	2.26	0.58
17:g:189:GLN:NE2	17:g:216:LYS:O	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:304:NEX:H241	25:p:308:CLA:H2	1.84	0.58
24:q:310:CHL:HBB1	24:q:310:CHL:HHC	1.85	0.58
13:s:128:ARG:NH2	13:s:229:LEU:O	2.36	0.58
25:r:311:CLA:H2A	25:r:311:CLA:HED3	1.85	0.58
8:R:135:ARG:HD3	25:R:609:CLA:C4C	2.33	0.58
13:S:180:ASN:ND2	24:S:605:CHL:OBD	2.35	0.58
19:A:270:SER:OG	32:A:609:SQD:O49	2.21	0.58
12:u:53:PRO:HG3	12:u:67:ASP:HB3	1.86	0.58
12:u:118:TRP:HE1	12:u:219:ALA:HB2	1.67	0.58
24:9:309:CHL:HHC	24:9:309:CHL:HBB1	1.86	0.57
20:C:295:PRO:HB3	20:C:346:PHE:HB3	1.86	0.57
28:6:303:NEX:C30	24:6:309:CHL:H3A	2.33	0.57
20:c:295:PRO:HB3	20:c:346:PHE:HB3	1.86	0.57
21:d:189:HIS:HA	21:d:294:ARG:HD3	1.84	0.57
10:1:198:TRP:HE1	24:1:317:CHL:HMC	1.69	0.57
18:B:71:ILE:HD11	25:B:607:CLA:H2A	1.87	0.57
12:6:84:LEU:O	12:6:88:HIS:ND1	2.36	0.57
28:g:304:NEX:H362	25:g:308:CLA:CHC	2.35	0.57
8:R:213:ASP:OD1	26:R:614:0IE:O42	2.21	0.57
24:1:309:CHL:HBC2	24:1:310:CHL:HHD	1.87	0.57
28:S:617:NEX:H383	25:8:306:CLA:C3B	2.34	0.57
24:Y:304:CHL:HHC	24:Y:304:CHL:HBB1	1.85	0.57
19:A:162:PRO:HB3	19:A:168:PHE:HA	1.86	0.57
10:4:168:LYS:HD3	25:4:315:CLA:HAA2	1.85	0.57
12:p:239:ASN:ND2	12:p:240:ASN:OD1	2.35	0.57
17:G:8:ARG:NH2	17:G:31:ASP:OD1	2.38	0.57
12:9:100:LEU:O	12:9:104:LEU:N	2.27	0.57
18:B:372:ASP:OD1	18:B:373:ASP:N	2.33	0.57
12:6:221:VAL:HG23	12:6:222:THR:HG23	1.87	0.57
12:6:230:TRP:HE1	24:6:317:CHL:HMC	1.69	0.57
17:g:209:ASN:HD22	17:n:114:LEU:HD21	1.69	0.57
12:u:90:ARG:NE	12:u:201:GLU:OE2	2.29	0.57
24:u:310:CHL:HBC2	24:u:311:CHL:HHD	1.86	0.57
12:p:162:TYR:HB3	24:p:312:CHL:HMC	1.86	0.57
12:p:233:HIS:CG	25:p:317:CLA:HAA2	2.40	0.57
20:c:395:VAL:HG21	20:c:404:ALA:HB3	1.85	0.57
12:3:178:PRO:HD3	24:3:311:CHL:HMD1	1.86	0.57
11:5:8:ARG:NH1	11:5:31:ASP:O	2.33	0.57
28:7:304:NEX:H222	25:7:308:CLA:NC	2.19	0.57
17:G:19:ALA:HB2	17:N:132:CYS:HB3	1.86	0.57
12:9:166:GLY:HA3	12:9:172:PRO:HD3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:57:ALA:HB1	17:N:173:GLY:HA3	1.86	0.57
17:8:85:VAL:HG23	17:8:88:LYS:HB2	1.86	0.57
18:b:53:ASN:ND2	18:b:58:GLN:OE1	2.37	0.57
8:r:160:GLU:OE2	8:r:164:GLN:NE2	2.34	0.57
4:I:27:ASP:OD1	19:A:136:ARG:NH2	2.37	0.57
15:V:300:LEU:HA	15:V:303:ARG:HB2	1.87	0.57
28:6:303:NEX:C26	24:6:309:CHL:HAA1	2.35	0.57
17:g:58:ARG:HA	17:g:61:MET:HE3	1.86	0.57
12:9:168:PRO:HG3	28:9:319:NEX:H192	1.86	0.57
25:9:306:CLA:H12	17:N:39:LEU:HD11	1.85	0.57
17:g:168:LYS:O	17:g:172:ASN:ND2	2.27	0.57
18:b:341:LEU:HD11	18:b:431:GLU:HB3	1.86	0.57
12:7:52:VAL:HG12	12:7:65:GLY:HA3	1.87	0.57
17:G:168:LYS:O	17:G:172:ASN:ND2	2.28	0.57
20:C:83:LEU:O	20:C:166:LYS:NZ	2.32	0.57
19:a:162:PRO:HB3	19:a:168:PHE:HA	1.87	0.57
19:a:299:GLY:O	20:c:391:SER:OG	2.21	0.57
8:R:73:SER:HB2	24:R:602:CHL:HAA2	1.87	0.57
17:G:21:PRO:HG2	17:G:35:ASP:HB3	1.86	0.57
17:N:24:LEU:HD22	17:N:33:GLY:HA2	1.85	0.57
23:f:201:HEM:HMC2	23:f:201:HEM:HBC2	1.86	0.57
11:5:171:LYS:NZ	30:5:319:LHG:O4	2.38	0.57
20:c:83:LEU:O	20:c:166:LYS:NZ	2.33	0.57
23:E:201:HEM:HBC2	23:E:201:HEM:HMC2	1.86	0.56
13:S:199:GLU:HG2	24:S:608:CHL:C1B	2.35	0.56
18:B:53:ASN:ND2	18:B:58:GLN:OE1	2.37	0.56
2:e:48:TYR:O	2:e:52:HIS:ND1	2.38	0.56
12:u:43:TRP:HB3	12:u:64:TYR:HB3	1.87	0.56
17:n:92:GLN:HE21	17:n:99:LEU:HG	1.70	0.56
25:b:614:CLA:H42	32:b:618:SQD:H122	1.87	0.56
25:B:604:CLA:H111	25:B:615:CLA:H42	1.86	0.56
28:4:303:NEX:O24	24:4:309:CHL:HAA1	2.05	0.56
8:r:246:PHE:CE1	25:r:313:CLA:HAC2	2.40	0.56
23:E:201:HEM:HMB2	23:E:201:HEM:HBB2	1.87	0.56
8:R:162:ILE:HG23	8:R:167:GLY:HA2	1.87	0.56
11:2:71:GLU:HA	11:2:84:SER:HB2	1.87	0.56
20:C:281:ASN:ND2	37:C:620:DGD:HE61	2.20	0.56
23:f:201:HEM:HBB2	23:f:201:HEM:HMB2	1.87	0.56
11:5:201:HIS:CG	25:5:317:CLA:HAA2	2.40	0.56
17:n:126:LEU:HB2	28:n:303:NEX:C20	2.34	0.56
17:q:54:LEU:HD23	17:q:144:LEU:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:15:ASP:HB3	18:b:18:ARG:HB2	1.87	0.56
18:b:71:ILE:HD11	25:b:607:CLA:H2A	1.87	0.56
17:G:58:ARG:HA	17:G:61:MET:HE3	1.87	0.56
10:4:198:TRP:HE1	24:4:317:CHL:HMC	1.70	0.56
12:6:178:PRO:HD3	24:6:311:CHL:HMD1	1.87	0.56
24:y:305:CHL:H52	24:q:311:CHL:HBB1	1.86	0.56
12:p:249:THR:H	12:p:252:ALA:HB2	1.71	0.56
6:l:14:ASN:OD1	6:l:14:ASN:N	2.39	0.56
17:q:57:ALA:HB1	17:q:173:GLY:HA3	1.86	0.56
28:7:304:NEX:H393	25:7:308:CLA:CAB	2.35	0.56
13:S:102:TYR:HB2	24:S:602:CHL:HMD3	1.88	0.56
17:g:83:GLU:N	17:g:92:GLN:OE1	2.38	0.56
17:g:118:TRP:HZ2	24:u:318:CHL:HBD	1.71	0.56
25:b:604:CLA:H111	25:b:615:CLA:H42	1.87	0.56
17:8:57:ALA:HB1	17:8:173:GLY:HA3	1.86	0.56
17:n:57:ALA:HB1	17:n:173:GLY:HA3	1.87	0.56
28:7:304:NEX:C38	25:7:308:CLA:CHB	2.84	0.56
18:B:480:ALA:HB1	19:A:229:GLU:HA	1.88	0.56
13:s:240:LEU:HD23	25:s:410:CLA:H11	1.86	0.56
8:r:162:ILE:HG23	8:r:167:GLY:HA2	1.88	0.56
12:3:190:ASP:HB3	12:3:193:THR:HG22	1.87	0.56
13:S:122:PHE:O	13:S:126:HIS:ND1	2.31	0.56
24:6:309:CHL:HBC2	24:6:310:CHL:HHD	1.88	0.56
15:v:300:LEU:HA	15:v:303:ARG:HB2	1.87	0.56
25:a:605:CLA:HAB	25:d:404:CLA:H51	1.88	0.56
11:2:201:HIS:CG	25:2:317:CLA:HAA2	2.41	0.56
15:V:282:GLN:HG2	15:V:283:LEU:H	1.71	0.56
17:Y:201:HIS:CG	25:Y:316:CLA:HAA2	2.42	0.56
17:8:54:LEU:HD23	17:8:144:LEU:HB3	1.87	0.56
18:B:153:PHE:O	18:B:158:VAL:HG23	2.06	0.56
30:A:601:LHG:H152	39:D:406:PL9:H252	1.86	0.56
22:W:96:TRP:CH2	33:W:201:LMG:H112	2.41	0.56
17:g:19:ALA:HB2	17:n:132:CYS:HB3	1.88	0.56
18:b:278:GLY:O	18:b:281:ALA:N	2.38	0.56
13:s:199:GLU:HG2	24:s:409:CHL:C1B	2.36	0.56
24:3:309:CHL:HAA2	28:3:318:NEX:O24	2.03	0.55
24:y:305:CHL:HHC	24:y:305:CHL:HBB1	1.88	0.55
18:b:276:ASP:N	18:b:276:ASP:OD1	2.24	0.55
13:s:209:LYS:NZ	13:s:220:SER:OG	2.31	0.55
10:1:61:MET:SD	25:1:313:CLA:HAB	2.46	0.55
13:S:70:LYS:HE2	13:S:77:ALA:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:9:43:TRP:HB3	12:9:64:TYR:HB3	1.87	0.55
17:Y:51:GLU:HA	17:Y:144:LEU:HD21	1.89	0.55
17:Y:128:GLU:HA	17:Y:131:ARG:HG2	1.88	0.55
12:6:89:SER:HB2	12:6:205:GLY:HA3	1.87	0.55
17:g:104:ASN:HB3	17:g:107:LEU:HD23	1.88	0.55
17:y:125:GLY:HA2	24:y:313:CHL:HAB	1.87	0.55
19:a:143:ILE:HG12	21:d:220:ASN:HD22	1.72	0.55
8:R:67:PHE:CE2	27:R:615:XAT:H383	2.29	0.55
19:A:143:ILE:HG12	21:D:220:ASN:HD22	1.71	0.55
17:g:55:ILE:HG13	17:g:131:ARG:HH21	1.70	0.55
17:g:104:ASN:ND2	17:g:106:SER:OG	2.38	0.55
28:p:304:NEX:C36	25:p:308:CLA:CHC	2.83	0.55
11:2:171:LYS:NZ	30:2:319:LHG:O4	2.39	0.55
13:S:76:ARG:NH1	13:S:101:ASP:O	2.40	0.55
17:G:209:ASN:HD22	17:N:114:LEU:HD21	1.71	0.55
18:B:340:TRP:CD1	18:B:342:GLY:H	2.25	0.55
12:6:117:VAL:HG23	12:6:120:SER:HB2	1.88	0.55
12:6:190:ASP:HB3	12:6:193:THR:HG22	1.87	0.55
25:u:307:CLA:H12	17:n:39:LEU:HD11	1.88	0.55
28:n:303:NEX:O24	25:n:307:CLA:H43	2.07	0.55
18:b:155:ALA:O	18:b:159:THR:OG1	2.23	0.55
13:s:122:PHE:O	13:s:126:HIS:ND1	2.34	0.55
6:L:34:SER:OG	19:A:76:ASN:ND2	2.39	0.55
13:S:99:PRO:HG2	13:S:120:ARG:HH22	1.70	0.55
24:Y:304:CHL:H52	24:8:310:CHL:HBB1	1.88	0.55
19:A:133:LEU:HD23	21:D:256:ILE:HG12	1.87	0.55
28:s:401:NEX:O3	25:s:411:CLA:CGA	2.54	0.55
28:1:303:NEX:H362	25:1:307:CLA:CHC	2.36	0.55
15:v:299:LEU:O	15:v:303:ARG:N	2.32	0.55
24:g:306:CHL:H93	25:g:307:CLA:HHB	1.88	0.55
12:3:84:LEU:O	12:3:88:HIS:ND1	2.39	0.55
17:N:130:TYR:HB3	24:N:311:CHL:CMC	2.37	0.55
24:N:304:CHL:HMD1	30:N:318:LHG:H251	1.88	0.55
17:n:68:LEU:HD13	17:n:195:VAL:HG22	1.87	0.55
24:n:304:CHL:HMD1	30:n:318:LHG:H251	1.89	0.55
17:G:83:GLU:N	17:G:92:GLN:OE1	2.39	0.55
17:Y:125:GLY:HA2	24:Y:312:CHL:HAB	1.88	0.55
24:4:309:CHL:HBC2	24:4:310:CHL:HHD	1.89	0.55
17:n:130:TYR:HB3	24:n:311:CHL:CMC	2.36	0.55
20:c:448:ASP:O	20:c:449:ARG:HB2	2.07	0.55
25:r:305:CLA:HMB1	24:r:306:CHL:HBB1	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:61:MET:SD	25:4:313:CLA:HAB	2.46	0.55
17:y:201:HIS:CG	25:y:317:CLA:HAA2	2.41	0.55
25:c:603:CLA:H203	25:c:610:CLA:HAB	1.87	0.55
8:r:186:VAL:HG23	24:r:309:CHL:HBB2	1.87	0.55
8:R:69:PRO:C	8:R:71:CYS:H	2.15	0.55
25:R:604:CLA:C2B	28:R:616:NEX:H383	2.37	0.55
11:5:71:GLU:HA	11:5:84:SER:HB2	1.87	0.55
19:a:133:LEU:HD23	21:d:256:ILE:HG12	1.88	0.55
18:B:341:LEU:HD11	18:B:431:GLU:HB3	1.87	0.54
20:C:448:ASP:O	20:C:449:ARG:HB2	2.07	0.54
3:h:51:VAL:HG21	25:d:405:CLA:H43	1.89	0.54
28:4:303:NEX:H362	25:4:307:CLA:HAB	1.85	0.54
18:b:340:TRP:CD1	18:b:342:GLY:H	2.25	0.54
25:b:604:CLA:HBA2	25:b:606:CLA:H151	1.89	0.54
20:c:395:VAL:HG23	20:c:407:PHE:N	2.22	0.54
17:G:51:GLU:HA	17:G:144:LEU:HD21	1.89	0.54
17:G:55:ILE:HG13	17:G:131:ARG:HH21	1.70	0.54
17:G:110:ALA:HA	24:G:309:CHL:HHC	1.90	0.54
28:G:304:NEX:C15	24:G:312:CHL:HMB3	2.36	0.54
12:9:86:VAL:HB	12:9:176:LEU:HD22	1.89	0.54
17:8:24:LEU:HD11	17:8:35:ASP:HB2	1.90	0.54
19:A:192:ILE:HG13	19:A:293:MET:HE1	1.89	0.54
12:6:239:ASN:HA	12:6:244:THR:HG21	1.89	0.54
28:6:303:NEX:C31	24:6:309:CHL:H3A	2.38	0.54
24:y:305:CHL:H62	30:y:319:LHG:H181	1.89	0.54
24:p:310:CHL:HBC2	24:p:311:CHL:HHD	1.88	0.54
17:q:92:GLN:HB2	17:q:99:LEU:HD12	1.89	0.54
25:b:609:CLA:H112	25:b:612:CLA:H72	1.88	0.54
3:H:23:ASN:ND2	18:B:122:LEU:O	2.39	0.54
17:G:32:TYR:HB2	24:G:306:CHL:HMD1	1.89	0.54
18:B:121:GLU:OE1	18:B:121:GLU:N	2.41	0.54
6:l:34:SER:OG	19:a:76:ASN:ND2	2.39	0.54
17:g:8:ARG:NH2	17:g:31:ASP:OD1	2.39	0.54
17:q:51:GLU:HA	17:q:144:LEU:HD11	1.90	0.54
18:b:121:GLU:OE1	18:b:121:GLU:N	2.40	0.54
20:c:281:ASN:ND2	37:c:619:DGD:HE61	2.21	0.54
12:9:200:LYS:HD2	25:9:315:CLA:HBD	1.90	0.54
17:N:51:GLU:HA	17:N:144:LEU:HD11	1.89	0.54
24:4:312:CHL:HMB3	24:5:305:CHL:HHB	1.88	0.54
12:p:41:ALA:HB1	24:p:305:CHL:HBC1	1.89	0.54
30:a:601:LHG:H152	39:d:406:PL9:H252	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:604:CLA:HBA2	25:B:606:CLA:H151	1.89	0.54
6:l:20:TRP:CE2	30:d:407:LHG:H241	2.43	0.54
17:g:21:PRO:HG2	17:g:35:ASP:HB3	1.88	0.54
12:p:163:ARG:NH2	24:p:313:CHL:O1D	2.41	0.54
8:r:214:PRO:O	28:r:301:NEX:O3	2.25	0.54
2:E:78:SER:HA	21:D:56:THR:HG21	1.90	0.54
8:R:208:PRO:HB3	24:R:607:CHL:HBC2	1.89	0.54
17:G:222:ILE:HG21	17:N:188:LEU:HD12	1.89	0.54
18:B:57:ARG:NH2	18:B:334:ASP:OD1	2.39	0.54
25:B:603:CLA:HAB	25:B:605:CLA:H152	1.90	0.54
25:C:603:CLA:H203	25:C:610:CLA:HAB	1.89	0.54
12:p:165:SER:OG	17:q:17:GLU:O	2.22	0.54
12:p:200:LYS:HD3	25:p:316:CLA:HAA2	1.88	0.54
25:q:306:CLA:C2B	28:s:401:NEX:H383	2.38	0.54
19:a:85:THR:HA	19:a:109:GLY:HA3	1.90	0.54
12:u:200:LYS:NZ	25:u:316:CLA:O1A	2.41	0.54
20:c:332:SER:OG	20:c:336:GLU:OE1	2.26	0.54
13:s:102:TYR:HB2	24:s:403:CHL:HMD3	1.88	0.54
25:r:305:CLA:C4B	28:r:317:NEX:H222	2.38	0.54
12:7:169:LEU:O	12:7:181:SER:OG	2.22	0.54
3:H:51:VAL:HG21	25:D:405:CLA:H43	1.89	0.54
11:2:189:GLN:NE2	26:2:303:0IE:O40	2.41	0.54
13:S:93:TYR:OH	13:S:105:ASP:OD2	2.26	0.54
17:Y:168:LYS:HD3	25:Y:315:CLA:HAA2	1.90	0.54
10:4:30:GLY:HA3	10:4:170:ILE:HD13	1.90	0.54
17:n:79:VAL:HG21	17:n:102:LEU:HD12	1.90	0.54
18:b:480:ALA:HB1	19:a:229:GLU:HA	1.90	0.54
13:s:57:GLY:H	13:s:64:ASN:H	1.54	0.54
13:s:115:ASN:O	13:s:118:THR:OG1	2.26	0.54
3:H:48:VAL:O	3:H:52:ILE:HG12	2.08	0.54
13:S:224:ASP:OD1	13:S:224:ASP:N	2.39	0.54
32:B:618:SQD:H321	16:t:50:GLY:HA3	1.89	0.54
28:p:304:NEX:H241	25:p:308:CLA:C2	2.37	0.54
8:R:246:PHE:CE1	25:R:612:CLA:HAC2	2.42	0.54
17:8:145:TYR:HB3	25:8:311:CLA:HED2	1.90	0.54
12:u:240:ASN:HD22	25:u:317:CLA:HED1	1.72	0.54
17:y:51:GLU:HA	17:y:144:LEU:HD21	1.89	0.54
12:p:169:LEU:O	12:p:181:SER:OG	2.21	0.54
19:a:307:VAL:HG12	19:a:313:VAL:HA	1.90	0.54
6:L:20:TRP:CE2	30:D:407:LHG:H241	2.43	0.53
7:M:26:TYR:O	7:M:30:ALA:N	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:209:LYS:NZ	13:S:220:SER:OG	2.29	0.53
12:9:61:PRO:HB2	12:9:202:ILE:HD12	1.90	0.53
12:9:74:ASP:HB3	12:9:77:MET:HG2	1.90	0.53
12:9:166:GLY:HA2	24:9:311:CHL:HMC	1.90	0.53
25:B:609:CLA:H112	25:B:612:CLA:H72	1.90	0.53
18:b:58:GLN:HB2	18:b:60:MET:HE3	1.90	0.53
20:c:357:LEU:HA	20:c:367:LYS:HG2	1.90	0.53
13:s:70:LYS:HE2	13:s:77:ALA:HB2	1.90	0.53
11:2:61:MET:SD	25:2:314:CLA:HAB	2.48	0.53
12:9:113:LEU:HB3	12:9:116:PRO:HB3	1.89	0.53
19:A:307:VAL:HG12	19:A:313:VAL:HA	1.91	0.53
20:C:257:GLU:OE1	20:C:435:ARG:NH1	2.38	0.53
20:C:357:LEU:HA	20:C:367:LYS:HG2	1.89	0.53
17:g:57:ALA:HB1	17:g:173:GLY:HA3	1.90	0.53
12:u:115:SER:HB2	12:u:120:SER:HB3	1.90	0.53
20:c:385:THR:HG1	20:c:386:HIS:HD1	1.55	0.53
8:r:208:PRO:HB3	24:r:308:CHL:HBC2	1.90	0.53
28:7:304:NEX:C40	24:7:310:CHL:O2A	2.56	0.53
8:R:82:ASP:N	8:R:82:ASP:OD1	2.37	0.53
17:n:168:LYS:HD3	25:n:315:CLA:HAA2	1.90	0.53
19:a:319:ASP:O	19:a:322:ASN:ND2	2.41	0.53
10:1:57:ALA:HB1	10:1:173:GLY:HA3	1.90	0.53
17:Y:168:LYS:O	17:Y:172:ASN:ND2	2.27	0.53
18:B:464:PHE:HD2	25:B:611:CLA:HAC2	1.73	0.53
17:g:222:ILE:HG21	17:n:188:LEU:HD12	1.91	0.53
25:b:603:CLA:HAB	25:b:605:CLA:H152	1.90	0.53
20:c:315:ASN:HB3	20:c:318:SER:HB2	1.90	0.53
8:r:246:PHE:HD1	25:r:313:CLA:HMD3	1.72	0.53
10:1:142:ASP:OD2	10:1:145:TYR:N	2.37	0.53
11:2:47:ARG:HH22	11:2:48:ARG:HH21	1.57	0.53
20:C:315:ASN:HB3	20:C:318:SER:HB2	1.91	0.53
12:6:44:LEU:HD23	24:6:304:CHL:HHB	1.89	0.53
17:g:101:TYR:OH	28:g:304:NEX:O23	2.22	0.53
12:u:221:VAL:HG13	12:u:222:THR:HG23	1.90	0.53
17:n:143:PRO:HG2	17:n:144:LEU:HD22	1.90	0.53
24:q:308:CHL:CBA	28:s:401:NEX:H403	2.38	0.53
18:b:463:PHE:CZ	18:b:467:ILE:HD11	2.43	0.53
19:a:192:ILE:HG13	19:a:293:MET:HE1	1.91	0.53
20:c:332:SER:OG	20:c:336:GLU:N	2.41	0.53
13:s:76:ARG:NH1	13:s:101:ASP:O	2.41	0.53
13:s:93:TYR:OH	13:s:105:ASP:OD2	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:169:ASP:HA	13:s:179:ALA:HA	1.91	0.53
13:S:169:ASP:HA	13:S:179:ALA:HA	1.90	0.53
28:G:304:NEX:H362	25:G:308:CLA:C3B	2.38	0.53
11:5:61:MET:SD	25:5:314:CLA:HAB	2.48	0.53
12:6:124:GLN:O	12:6:127:SER:OG	2.25	0.53
12:u:45:GLY:HA3	24:u:305:CHL:HBB1	1.90	0.53
17:n:22:SER:O	17:n:24:LEU:N	2.40	0.53
18:b:393:GLU:HG2	18:b:414:PRO:HB3	1.91	0.53
12:3:68:THR:N	26:3:302:0IE:O42	2.41	0.53
12:9:129:GLY:O	12:9:143:GLN:NE2	2.36	0.53
2:e:78:SER:OG	21:d:54:PHE:O	2.27	0.53
3:h:54:LEU:HA	25:b:602:CLA:H43	1.90	0.53
10:4:142:ASP:OD2	10:4:145:TYR:N	2.38	0.53
17:g:109:HIS:O	17:g:111:GLN:NE2	2.41	0.53
18:b:275:TRP:CE2	18:b:315:ILE:HD13	2.44	0.53
2:E:88:ASP:OD1	2:E:88:ASP:N	2.40	0.53
12:3:79:LYS:NZ	12:3:80:GLN:OE1	2.42	0.53
28:G:304:NEX:H15	24:G:312:CHL:CMB	2.37	0.53
17:8:128:GLU:OE1	17:8:131:ARG:NH1	2.37	0.53
19:A:273:PHE:CE1	30:D:408:LHG:HC61	2.44	0.53
17:q:130:TYR:O	17:q:134:GLY:N	2.35	0.53
8:r:243:PHE:CE2	27:r:316:XAT:H10	2.44	0.53
8:R:258:PHE:HA	8:R:261:LEU:HB2	1.90	0.53
13:S:267:GLY:O	13:S:271:GLN:HG2	2.09	0.53
28:G:304:NEX:H362	25:G:308:CLA:CAB	2.38	0.53
12:9:35:TRP:NE1	12:9:64:TYR:OH	2.30	0.53
20:C:163:LEU:HD23	20:C:225:HIS:CD2	2.44	0.53
21:D:253:TRP:HB2	21:D:260:ALA:HB2	1.91	0.53
3:h:23:ASN:ND2	18:b:122:LEU:O	2.38	0.53
10:4:11:TRP:O	10:4:16:SER:OG	2.25	0.53
16:T:50:GLY:HA3	32:b:618:SQD:H321	1.91	0.52
17:N:62:LEU:HD12	25:N:307:CLA:HAB	1.92	0.52
20:C:142:LYS:HB3	20:C:244:PRO:HG2	1.91	0.52
20:C:395:VAL:HG21	20:C:404:ALA:HB3	1.90	0.52
20:C:408:VAL:H	37:C:619:DGD:C3E	2.22	0.52
12:u:131:ILE:HG13	24:u:310:CHL:HMD1	1.89	0.52
32:b:618:SQD:H292	32:b:618:SQD:H162	1.89	0.52
13:s:58:TRP:HE1	28:s:401:NEX:C19	2.10	0.52
8:r:213:ASP:O	8:r:216:ASN:ND2	2.42	0.52
13:S:59:PHE:HE2	28:S:617:NEX:HO3	0.68	0.52
12:9:92:ALA:O	12:9:96:THR:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:286:THR:OG1	25:A:603:CLA:O1D	2.26	0.52
20:C:257:GLU:OE2	20:C:432:HIS:ND1	2.36	0.52
6:l:5:ASN:HD22	18:b:18:ARG:CZ	2.23	0.52
12:p:89:SER:HB2	12:p:205:GLY:HA3	1.91	0.52
20:c:408:VAL:H	37:c:618:DGD:C3E	2.22	0.52
24:1:312:CHL:HMB3	24:2:305:CHL:HHB	1.92	0.52
12:3:91:TRP:O	26:3:302:0IE:O29	2.28	0.52
12:9:83:GLU:HA	12:9:176:LEU:HD21	1.90	0.52
26:9:303:0IE:O42	30:9:318:LHG:O2	2.28	0.52
18:B:58:GLN:HB2	18:B:60:MET:HE3	1.91	0.52
21:D:141:TYR:O	21:D:142:ASN:C	2.52	0.52
28:6:303:NEX:C29	24:6:309:CHL:H3A	2.40	0.52
17:g:52:LEU:O	17:g:56:HIS:ND1	2.42	0.52
18:b:198:ILE:HG23	18:b:202:HIS:HE1	1.74	0.52
8:r:135:ARG:NH1	24:r:308:CHL:OBD	2.38	0.52
8:R:76:VAL:O	8:R:104:THR:OG1	2.27	0.52
20:C:337:ILE:HG22	20:C:363:LEU:HB2	1.92	0.52
18:b:464:PHE:HD2	25:b:611:CLA:HAC2	1.73	0.52
24:1:310:CHL:HHC	24:1:310:CHL:HBB1	1.90	0.52
28:G:304:NEX:C14	24:G:312:CHL:HMB1	2.40	0.52
19:A:85:THR:HA	19:A:109:GLY:HA3	1.91	0.52
21:d:253:TRP:HB2	21:d:260:ALA:HB2	1.92	0.52
12:9:115:SER:HB2	12:9:120:SER:HB3	1.91	0.52
17:N:61:MET:HG3	17:N:173:GLY:HA2	1.92	0.52
17:8:21:PRO:HG2	17:8:35:ASP:HB3	1.91	0.52
18:B:198:ILE:HG23	18:B:202:HIS:HE1	1.74	0.52
20:C:395:VAL:HG23	20:C:407:PHE:H	1.75	0.52
17:g:171:LYS:NZ	25:g:315:CLA:O1D	2.37	0.52
21:d:113:PHE:O	21:d:117:HIS:ND1	2.39	0.52
8:r:69:PRO:HG2	27:r:316:XAT:H221	1.91	0.52
8:R:107:ASP:OD1	8:R:107:ASP:N	2.40	0.52
17:8:151:ASP:OD1	29:8:301:0UR:O40	2.28	0.52
20:C:332:SER:OG	20:C:336:GLU:OE1	2.26	0.52
13:s:58:TRP:NE1	28:s:401:NEX:H181	2.25	0.52
17:g:217:PHE:CD1	24:n:310:CHL:H2	2.44	0.52
12:p:133:TYR:CE1	28:p:304:NEX:O23	2.56	0.52
12:p:148:ILE:HG12	24:p:309:CHL:HAC1	1.90	0.52
28:1:303:NEX:C31	24:1:309:CHL:CBA	2.86	0.52
11:2:99:LEU:HD21	25:2:308:CLA:HAA2	1.92	0.52
11:2:189:GLN:NE2	11:2:218:LYS:O	2.43	0.52
17:G:130:TYR:OH	28:G:304:NEX:C19	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:304:NEX:C13	24:G:312:CHL:HMB1	2.39	0.52
12:9:226:PRO:O	29:9:301:0UR:O39	2.28	0.52
18:B:477:ASP:OD1	18:B:477:ASP:N	2.36	0.52
20:C:202:LEU:HB3	22:W:76:ALA:H	1.74	0.52
20:C:332:SER:OG	20:C:336:GLU:N	2.41	0.52
7:m:26:TYR:O	7:m:30:ALA:N	2.42	0.52
10:4:168:LYS:NZ	25:4:315:CLA:O1A	2.41	0.52
17:g:101:TYR:HE2	28:g:304:NEX:H1	1.56	0.52
17:g:110:ALA:HA	24:g:309:CHL:HHC	1.91	0.52
12:u:229:ASN:ND2	25:u:317:CLA:O1D	2.42	0.52
17:q:8:ARG:NE	17:q:31:ASP:O	2.35	0.52
3:H:52:ILE:HD12	14:X:79:LEU:HD21	1.91	0.52
13:S:115:ASN:O	13:S:118:THR:OG1	2.25	0.52
17:G:57:ALA:HB1	17:G:173:GLY:HA3	1.92	0.52
17:8:51:GLU:HA	17:8:144:LEU:HD11	1.92	0.52
17:8:130:TYR:O	17:8:134:GLY:N	2.35	0.52
18:B:393:GLU:HG2	18:B:414:PRO:HB3	1.92	0.52
25:A:607:CLA:HAA2	33:C:618:LMG:H111	1.92	0.52
17:y:145:TYR:HB3	25:y:314:CLA:HED2	1.92	0.52
18:b:54:PRO:HD2	18:b:57:ARG:HB2	1.92	0.52
20:c:163:LEU:HD23	20:c:225:HIS:CD2	2.45	0.52
24:s:407:CHL:HHC	24:s:407:CHL:HBB1	1.92	0.52
3:H:54:LEU:HA	25:B:602:CLA:H43	1.92	0.51
21:D:152:VAL:HG21	21:D:279:LEU:HD13	1.91	0.51
17:g:120:GLN:OE1	24:g:311:CHL:HMC	2.10	0.51
12:p:40:ARG:NE	12:p:63:ASP:OD1	2.43	0.51
24:q:308:CHL:HHC	24:q:308:CHL:HBB1	1.92	0.51
19:a:225:ARG:H	19:a:225:ARG:HD2	1.75	0.51
2:E:80:ARG:H	2:E:83:GLU:HB2	1.74	0.51
8:R:68:ASP:HA	27:R:615:XAT:O23	2.10	0.51
19:A:233:THR:OG1	30:A:612:LHG:O1	2.28	0.51
11:5:8:ARG:NH1	11:5:31:ASP:OD1	2.43	0.51
11:5:99:LEU:HD21	25:5:308:CLA:HAA2	1.92	0.51
28:6:303:NEX:H241	25:6:307:CLA:HBA2	1.92	0.51
12:u:117:VAL:HG13	12:u:118:TRP:H	1.74	0.51
17:y:206:VAL:O	17:y:209:ASN:ND2	2.43	0.51
24:p:305:CHL:C1D	30:p:319:LHG:HC82	2.41	0.51
13:s:108:GLY:O	13:s:111:LYS:HG3	2.11	0.51
12:7:76:GLU:O	12:7:80:GLN:NE2	2.43	0.51
8:R:163:LEU:HB2	24:R:606:CHL:HMD1	1.93	0.51
28:1:303:NEX:H15	24:1:311:CHL:HMB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:45:THR:HA	12:9:70:GLY:HA3	1.93	0.51
20:C:261:SER:O	20:C:429:HIS:ND1	2.43	0.51
2:e:88:ASP:OD1	2:e:88:ASP:N	2.38	0.51
28:5:304:NEX:H172	17:n:152:PRO:HB2	1.92	0.51
17:y:59:TRP:CE2	24:y:312:CHL:HED2	2.45	0.51
18:b:480:ALA:H	21:d:139:ARG:NH1	2.08	0.51
12:7:89:SER:HB2	12:7:205:GLY:HA3	1.92	0.51
10:1:51:GLU:HA	10:1:144:LEU:HD21	1.92	0.51
28:S:617:NEX:C14	17:8:123:LEU:HD22	2.39	0.51
12:u:200:LYS:HD2	25:u:316:CLA:HBD	1.93	0.51
20:c:261:SER:O	20:c:429:HIS:ND1	2.43	0.51
20:c:337:ILE:HG22	20:c:363:LEU:HB2	1.92	0.51
13:s:224:ASP:N	13:s:224:ASP:OD1	2.38	0.51
13:s:267:GLY:O	13:s:271:GLN:HG2	2.09	0.51
8:r:67:PHE:HE2	27:r:316:XAT:H383	1.74	0.51
8:r:69:PRO:C	8:r:71:CYS:H	2.16	0.51
8:r:107:ASP:OD1	8:r:107:ASP:N	2.42	0.51
10:1:100:ASP:OD2	10:1:109:HIS:ND1	2.32	0.51
8:r:245:GLY:O	8:r:249:GLN:N	2.39	0.51
11:2:185:VAL:HA	11:2:188:ILE:HB	1.91	0.51
18:B:275:TRP:CE2	18:B:315:ILE:HD13	2.46	0.51
18:B:397:VAL:HG23	18:B:417:VAL:HG11	1.93	0.51
17:q:151:ASP:OD1	29:q:301:0UR:O40	2.28	0.51
17:G:217:PHE:CD1	24:N:310:CHL:H2	2.46	0.51
28:6:303:NEX:H31	24:6:309:CHL:CBA	2.40	0.51
12:u:226:PRO:O	29:u:301:0UR:O39	2.28	0.51
1:Z:1:MET:HB2	1:Z:4:LEU:HB3	1.92	0.51
8:R:135:ARG:NH1	24:R:607:CHL:OBD	2.38	0.51
12:9:93:MET:SD	25:9:313:CLA:HAB	2.51	0.51
17:Y:59:TRP:CE2	24:Y:311:CHL:HED2	2.45	0.51
18:B:379:ALA:HB2	18:B:395:VAL:HG21	1.93	0.51
12:u:209:MET:HB2	24:u:306:CHL:OMC	2.11	0.51
20:c:265:ALA:HB2	20:c:429:HIS:CG	2.46	0.51
12:7:145:ILE:HG23	12:7:146:LEU:HD12	1.93	0.51
8:R:67:PHE:HE2	27:R:615:XAT:C38	2.17	0.51
11:2:8:ARG:NH1	11:2:31:ASP:OD1	2.44	0.51
18:B:237:VAL:HG22	25:B:606:CLA:HMD1	1.93	0.51
17:g:54:LEU:HD23	17:g:144:LEU:HB3	1.93	0.51
17:q:85:VAL:HG23	17:q:88:LYS:HB2	1.93	0.51
18:b:57:ARG:NH2	18:b:334:ASP:OD1	2.40	0.51
12:7:166:GLY:HA2	24:7:312:CHL:HMC	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:117:TYR:OH	8:R:128:GLU:OE1	2.25	0.51
30:N:318:LHG:H272	30:N:318:LHG:HC62	1.92	0.51
17:Y:9:ALA:HB1	24:Y:304:CHL:HBC1	1.93	0.51
25:B:608:CLA:H2	33:B:619:LMG:H161	1.92	0.51
21:D:210:LEU:HD21	39:D:406:PL9:H13	1.92	0.51
17:q:192:LYS:NZ	17:q:200:GLU:OE2	2.38	0.51
18:b:272:ARG:NH1	18:b:276:ASP:OD2	2.44	0.51
2:E:79:PRO:CD	21:D:56:THR:HG21	2.40	0.50
25:R:604:CLA:CHC	28:R:616:NEX:H362	2.41	0.50
10:1:21:PRO:HG3	10:1:35:ASP:HB3	1.93	0.50
17:N:25:THR:OG1	17:N:27:GLU:OE1	2.24	0.50
17:Y:24:LEU:HD11	17:Y:35:ASP:HB2	1.94	0.50
25:C:604:CLA:CAA	37:C:619:DGD:HD61	2.41	0.50
21:D:252:PHE:CG	21:D:252:PHE:O	2.64	0.50
24:4:310:CHL:HHC	24:4:310:CHL:HBB1	1.92	0.50
17:g:45:THR:HA	12:u:70:GLY:HA3	1.93	0.50
17:g:93:ILE:HG21	17:g:113:ILE:HD12	1.93	0.50
17:y:189:GLN:NE2	17:y:213:TYR:O	2.44	0.50
24:q:310:CHL:CMA	28:s:401:NEX:H30	2.41	0.50
18:b:474:ILE:HD11	25:b:612:CLA:HAA2	1.91	0.50
20:c:336:GLU:OE1	20:c:336:GLU:N	2.43	0.50
12:7:133:TYR:HH	28:7:304:NEX:C23	2.23	0.50
20:C:118:VAL:HG21	25:C:611:CLA:H152	1.92	0.50
28:g:304:NEX:H362	25:g:308:CLA:C3B	2.40	0.50
18:b:397:VAL:HG23	18:b:417:VAL:HG11	1.93	0.50
21:d:39:PRO:HB2	25:d:405:CLA:HAB	1.94	0.50
21:d:141:TYR:O	21:d:142:ASN:C	2.51	0.50
13:s:99:PRO:HG2	13:s:120:ARG:HH22	1.76	0.50
6:L:5:ASN:HD22	18:B:18:ARG:CZ	2.24	0.50
18:B:154:GLY:HA2	18:B:158:VAL:CG2	2.42	0.50
19:A:283:ILE:HA	19:A:286:THR:HG22	1.92	0.50
12:6:91:TRP:O	26:6:302:0IE:O29	2.29	0.50
12:u:74:ASP:HB3	12:u:77:MET:HG2	1.94	0.50
18:b:237:VAL:HG22	25:b:606:CLA:HMD1	1.94	0.50
18:b:362:PHE:O	21:d:294:ARG:NH2	2.45	0.50
24:7:305:CHL:C1D	30:7:319:LHG:HC82	2.41	0.50
10:1:79:VAL:HG11	10:1:102:LEU:HD12	1.93	0.50
17:G:133:SER:HB3	12:9:50:GLY:H	1.76	0.50
12:9:55:TYR:OH	12:9:67:ASP:OD2	2.20	0.50
25:Y:314:CLA:H43	33:W:201:LMG:C10	2.42	0.50
18:B:54:PRO:HD2	18:B:57:ARG:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:392:ILE:HB	18:B:397:VAL:HG22	1.93	0.50
20:C:385:THR:HG1	20:C:386:HIS:HD1	1.59	0.50
28:n:303:NEX:O24	25:n:307:CLA:C4	2.59	0.50
17:q:145:TYR:HB3	25:q:312:CLA:HED2	1.94	0.50
18:b:23:HIS:ND1	25:b:615:CLA:OBD	2.44	0.50
18:b:256:MET:HA	18:b:263:THR:HG21	1.94	0.50
21:d:252:PHE:O	21:d:252:PHE:CG	2.64	0.50
11:2:214:ASP:N	11:2:214:ASP:OD1	2.43	0.50
24:3:309:CHL:H3A	28:3:318:NEX:C30	2.41	0.50
15:V:299:LEU:O	15:V:303:ARG:N	2.33	0.50
15:V:304:ASP:N	15:V:304:ASP:OD1	2.44	0.50
17:Y:206:VAL:O	17:Y:209:ASN:ND2	2.42	0.50
24:Y:309:CHL:HBA2	28:r:301:NEX:H403	1.94	0.50
17:8:45:THR:HG22	17:8:49:ASN:HD21	1.77	0.50
18:B:22:VAL:HG13	25:B:614:CLA:HMB2	1.94	0.50
20:C:265:ALA:HB2	20:C:429:HIS:CG	2.46	0.50
1:z:1:MET:SD	1:z:1:MET:N	2.80	0.50
10:4:134:GLY:HA2	24:4:311:CHL:HAC1	1.94	0.50
24:g:310:CHL:HBC2	24:g:311:CHL:HHD	1.92	0.50
12:u:248:ILE:HD12	12:u:252:ALA:HB3	1.94	0.50
8:r:243:PHE:CZ	27:r:316:XAT:H10	2.47	0.50
11:2:58:ARG:HA	11:2:61:MET:HE3	1.93	0.50
28:G:304:NEX:H222	25:G:308:CLA:C4B	2.41	0.50
18:B:480:ALA:H	21:D:139:ARG:NH1	2.06	0.50
3:h:48:VAL:O	3:h:52:ILE:HG12	2.12	0.50
33:i:101:LMG:HC71	20:c:204:SER:CB	2.41	0.50
11:5:214:ASP:N	11:5:214:ASP:OD1	2.43	0.50
12:p:245:ASP:OD1	12:p:245:ASP:N	2.33	0.50
17:q:21:PRO:HG2	17:q:35:ASP:HB3	1.93	0.50
18:b:357:ARG:HD3	18:b:371:LEU:HD11	1.93	0.50
19:a:174:LEU:HD22	35:a:606:PHO:H143	1.93	0.50
19:a:283:ILE:HA	19:a:286:THR:HG22	1.92	0.50
24:7:310:CHL:HBC2	24:7:311:CHL:HHD	1.93	0.50
8:R:57:LEU:HD11	8:R:68:ASP:HB2	1.93	0.50
13:S:57:GLY:H	13:S:64:ASN:H	1.60	0.50
13:S:58:TRP:CD2	17:8:136:PRO:HG3	2.46	0.50
13:S:120:ARG:HH21	13:S:124:LEU:HD12	1.77	0.50
12:9:83:GLU:HG2	12:9:176:LEU:HD21	1.93	0.50
17:8:92:GLN:HB2	17:8:99:LEU:HD12	1.93	0.50
25:B:604:CLA:H41	25:B:604:CLA:H92	1.93	0.50
19:A:174:LEU:HD22	35:A:606:PHO:H143	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:225:ARG:H	19:A:225:ARG:HD2	1.76	0.50
12:6:167:GLY:H	24:6:311:CHL:HMC	1.76	0.50
18:b:477:ASP:OD1	18:b:477:ASP:N	2.41	0.50
25:b:604:CLA:H41	25:b:604:CLA:H92	1.93	0.50
8:R:69:PRO:HD2	27:R:615:XAT:O23	2.12	0.50
18:B:151:PHE:HE1	18:B:203:ILE:HG23	1.76	0.50
18:B:474:ILE:HD11	25:B:612:CLA:HAA2	1.93	0.50
32:B:618:SQD:H292	32:B:618:SQD:H162	1.92	0.50
28:1:303:NEX:H383	25:1:307:CLA:CHB	2.41	0.50
12:3:117:VAL:HG23	12:3:120:SER:HB2	1.93	0.50
18:B:357:ARG:HD3	18:B:371:LEU:HD11	1.94	0.50
18:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.94	0.50
10:4:13:GLY:O	10:4:16:SER:OG	2.29	0.50
28:4:303:NEX:H383	25:4:307:CLA:C2B	2.41	0.50
12:6:191:PRO:HA	12:6:194:PHE:HB3	1.94	0.50
12:u:113:LEU:HB3	12:u:116:PRO:HB3	1.94	0.50
25:c:611:CLA:HBB1	25:c:611:CLA:HMB3	1.94	0.50
21:d:210:LEU:HD21	39:d:406:PL9:H13	1.92	0.50
12:7:93:MET:SD	25:7:314:CLA:HAB	2.52	0.50
10:1:65:VAL:O	10:1:69:THR:OG1	2.22	0.49
18:B:463:PHE:CZ	18:B:467:ILE:HD11	2.47	0.49
18:b:379:ALA:HB2	18:b:395:VAL:HG21	1.94	0.49
8:r:258:PHE:HA	8:r:261:LEU:HB2	1.94	0.49
2:E:78:SER:HA	21:D:56:THR:CG2	2.42	0.49
7:M:27:VAL:HG12	7:m:28:LYS:HB2	1.94	0.49
8:R:47:TRP:CE3	24:R:601:CHL:HAA1	2.47	0.49
8:R:48:MET:SD	17:N:136:PRO:HB3	2.51	0.49
8:R:169:TYR:N	8:R:172:LEU:O	2.43	0.49
21:D:126:MET:HE3	21:D:143:ALA:O	2.12	0.49
11:5:58:ARG:HA	11:5:61:MET:HE3	1.93	0.49
12:6:44:LEU:HB3	12:6:47:TYR:HB2	1.93	0.49
22:w:109:ASP:O	20:c:249:ARG:NH1	2.44	0.49
19:a:46:SER:O	19:a:50:ILE:HG13	2.12	0.49
19:a:103:ASP:O	19:a:104:GLU:C	2.54	0.49
19:a:233:THR:OG1	30:a:612:LHG:O1	2.30	0.49
8:r:53:ARG:NH1	8:r:64:ASP:OD2	2.44	0.49
12:7:40:ARG:NE	12:7:63:ASP:OD1	2.45	0.49
28:7:304:NEX:H241	25:7:308:CLA:C2	2.42	0.49
28:7:304:NEX:H382	25:7:308:CLA:HBA2	1.94	0.49
12:3:57:THR:OG1	12:3:59:GLU:OE1	2.23	0.49
12:9:83:GLU:HA	12:9:176:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:8:55:ILE:HG22	24:8:310:CHL:HMD2	1.93	0.49
17:8:83:GLU:O	17:8:92:GLN:NE2	2.45	0.49
24:8:309:CHL:HBB1	24:8:309:CHL:HHC	1.94	0.49
6:l:22:LEU:HB3	16:t:51:ILE:HD13	1.94	0.49
10:4:210:GLY:HA2	25:4:316:CLA:CAD	2.42	0.49
8:R:47:TRP:CD2	8:R:67:PHE:HD1	2.31	0.49
10:1:171:LYS:NZ	30:1:318:LHG:O5	2.44	0.49
11:2:151:ASP:OD1	29:2:301:0UR:O40	2.29	0.49
17:G:159:PRO:HA	17:G:162:PHE:HB3	1.94	0.49
12:9:233:HIS:CG	25:9:316:CLA:HAA2	2.47	0.49
17:N:69:THR:HG23	17:N:70:PRO:HD3	1.94	0.49
18:B:23:HIS:ND1	25:B:615:CLA:OBD	2.44	0.49
12:u:212:MET:HG2	26:u:302:0IE:C6	2.42	0.49
25:y:315:CLA:H43	33:w:201:LMG:C10	2.43	0.49
12:p:93:MET:SD	25:p:314:CLA:HAB	2.52	0.49
17:q:55:ILE:HG22	24:q:311:CHL:HMD2	1.93	0.49
18:b:392:ILE:HB	18:b:397:VAL:HG22	1.94	0.49
8:r:47:TRP:CE3	24:r:302:CHL:HAA1	2.48	0.49
28:7:304:NEX:C33	24:7:310:CHL:HBA1	2.42	0.49
3:H:67:ALA:HB3	3:H:72:SER:HB3	1.93	0.49
10:4:79:VAL:HG11	10:4:102:LEU:HD12	1.95	0.49
11:5:131:ARG:NH2	24:5:313:CHL:O1D	2.44	0.49
28:p:304:NEX:H403	24:p:310:CHL:O2A	2.12	0.49
18:b:22:VAL:HG13	25:b:614:CLA:HMB2	1.93	0.49
18:b:254:GLY:HA3	33:d:401:LMG:H132	1.95	0.49
18:b:372:ASP:N	18:b:376:ILE:O	2.39	0.49
6:L:22:LEU:HB3	16:T:51:ILE:HD13	1.95	0.49
12:3:233:HIS:CG	25:3:316:CLA:HAA2	2.47	0.49
13:S:131:MET:SD	25:S:609:CLA:HAB	2.53	0.49
12:9:80:GLN:HA	12:9:83:GLU:HB3	1.94	0.49
21:D:39:PRO:HB2	25:D:405:CLA:HAB	1.94	0.49
10:4:65:VAL:O	10:4:69:THR:OG1	2.22	0.49
11:5:108:ILE:HG13	25:5:308:CLA:H11	1.95	0.49
12:p:146:LEU:H	12:p:146:LEU:HD12	1.78	0.49
17:q:12:LEU:HD23	24:q:303:CHL:HHB	1.95	0.49
20:c:142:LYS:HB3	20:c:244:PRO:HG2	1.94	0.49
28:S:617:NEX:H403	24:8:308:CHL:CBA	2.42	0.49
17:G:88:LYS:HD3	24:G:311:CHL:HED2	1.95	0.49
12:9:43:TRP:NE1	12:9:51:ASP:OD2	2.45	0.49
12:9:206:ARG:HA	12:9:209:MET:HE2	1.95	0.49
28:N:303:NEX:O24	25:N:307:CLA:C4	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:426:LEU:HD13	18:B:443:PHE:HZ	1.78	0.49
10:4:51:GLU:HA	10:4:144:LEU:HD21	1.94	0.49
22:w:96:TRP:CZ3	33:w:201:LMG:HC91	2.48	0.49
20:c:175:ASP:OD2	20:c:185:ARG:NH2	2.40	0.49
8:R:231:ALA:O	8:R:235:HIS:ND1	2.42	0.49
17:8:164:GLU:HG2	17:8:168:LYS:HE3	1.95	0.49
18:B:8:VAL:HG23	18:B:9:HIS:CD2	2.48	0.49
6:l:24:LEU:HD13	30:a:601:LHG:H151	1.93	0.49
11:5:47:ARG:HH22	11:5:48:ARG:HH21	1.61	0.49
12:u:249:THR:H	12:u:252:ALA:HB2	1.78	0.49
12:p:84:LEU:HD11	17:q:37:ALA:HA	1.93	0.49
12:p:180:GLU:O	12:p:181:SER:OG	2.31	0.49
21:d:172:SER:HB2	21:d:177:ALA:HB1	1.95	0.49
24:8:308:CHL:HHC	24:8:308:CHL:HBB1	1.95	0.49
30:n:318:LHG:HC62	30:n:318:LHG:H272	1.95	0.49
13:s:295:LEU:O	13:s:299:ILE:HG13	2.13	0.49
25:R:604:CLA:C4B	28:R:616:NEX:H362	2.43	0.49
17:G:120:GLN:OE1	24:G:311:CHL:HMC	2.12	0.49
25:N:315:CLA:HED2	25:N:315:CLA:H2A	1.95	0.49
17:Y:55:ILE:HG22	24:Y:312:CHL:HMD2	1.95	0.49
19:A:137:LEU:HD22	20:C:454:VAL:HG22	1.94	0.49
19:A:253:GLY:O	19:A:257:ARG:HG2	2.12	0.49
1:z:5:PHE:HD1	1:z:57:LEU:HB3	1.78	0.49
12:u:92:ALA:O	12:u:96:THR:N	2.41	0.49
12:u:93:MET:SD	25:u:314:CLA:HAB	2.52	0.49
12:p:230:TRP:NE1	24:p:318:CHL:HMC	2.24	0.49
18:b:458:PHE:HB3	25:b:604:CLA:HBC2	1.94	0.49
19:a:170:ASP:OD2	20:c:345:ARG:NH1	2.42	0.49
21:d:126:MET:HE3	21:d:143:ALA:O	2.13	0.49
13:s:128:ARG:HD3	25:s:410:CLA:C4C	2.43	0.49
8:r:137:CYS:O	8:r:141:THR:HG22	2.13	0.49
12:7:180:GLU:O	12:7:181:SER:OG	2.30	0.49
8:R:137:CYS:O	8:R:141:THR:HG22	2.13	0.48
10:1:88:LYS:HD3	24:1:310:CHL:HED2	1.95	0.48
17:8:8:ARG:NE	17:8:31:ASP:O	2.31	0.48
17:8:37:ALA:HA	12:7:84:LEU:HD11	1.95	0.48
18:B:362:PHE:O	21:D:294:ARG:NH2	2.46	0.48
1:z:1:MET:HB2	1:z:4:LEU:HB3	1.95	0.48
2:e:90:GLN:OE1	19:a:312:ARG:NH1	2.46	0.48
17:n:61:MET:HG3	17:n:173:GLY:HA2	1.95	0.48
17:y:168:LYS:HD3	25:y:316:CLA:HAA2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:137:LEU:HD22	20:c:454:VAL:HG22	1.95	0.48
13:s:59:PHE:HD2	28:s:401:NEX:C18	2.23	0.48
8:r:57:LEU:HD11	8:r:68:ASP:HB2	1.95	0.48
1:Z:5:PHE:HD1	1:Z:57:LEU:HB3	1.78	0.48
25:R:612:CLA:HHB	24:N:308:CHL:HED1	1.95	0.48
13:S:108:GLY:O	13:S:111:LYS:HG3	2.13	0.48
28:N:303:NEX:O24	25:N:307:CLA:H43	2.13	0.48
20:C:336:GLU:OE1	20:C:336:GLU:N	2.43	0.48
12:p:56:LEU:HD11	12:p:67:ASP:HB2	1.95	0.48
28:p:304:NEX:H362	25:p:308:CLA:C3B	2.43	0.48
25:b:605:CLA:H8	25:b:606:CLA:H193	1.94	0.48
20:c:395:VAL:HG11	20:c:404:ALA:N	2.26	0.48
13:s:97:GLU:OE1	13:s:97:GLU:N	2.46	0.48
13:s:124:LEU:HD13	13:s:229:LEU:HB3	1.94	0.48
28:1:303:NEX:C36	25:1:307:CLA:CHC	2.91	0.48
12:3:230:TRP:HE1	24:3:317:CHL:HMC	1.78	0.48
28:G:304:NEX:H221	25:G:308:CLA:C1C	2.44	0.48
18:B:156:PHE:O	18:B:157:HIS:C	2.56	0.48
18:B:242:ILE:HG23	18:B:462:PHE:HD2	1.79	0.48
21:D:89:LEU:H	21:D:89:LEU:HG	1.41	0.48
4:i:27:ASP:OD1	19:a:136:ARG:NH2	2.41	0.48
8:r:169:TYR:N	8:r:172:LEU:O	2.46	0.48
12:7:56:LEU:HD11	12:7:67:ASP:HB2	1.95	0.48
9:F:14:THR:HG21	14:X:100:VAL:HG11	1.95	0.48
19:A:46:SER:O	19:A:50:ILE:HG13	2.12	0.48
24:u:306:CHL:HBB1	24:u:306:CHL:H51	1.95	0.48
3:H:26:TYR:CE2	8:R:83:ILE:HG12	2.48	0.48
8:R:243:PHE:CE2	27:R:615:XAT:H10	2.49	0.48
11:2:108:ILE:HG13	25:2:308:CLA:H11	1.95	0.48
17:G:54:LEU:HD12	17:G:144:LEU:HD13	1.95	0.48
17:N:65:VAL:O	17:N:69:THR:HG22	2.14	0.48
25:B:605:CLA:H8	25:B:606:CLA:H193	1.94	0.48
25:C:611:CLA:HBB1	25:C:611:CLA:HMB3	1.94	0.48
21:D:172:SER:HB2	21:D:177:ALA:HB1	1.95	0.48
17:g:164:GLU:O	17:g:167:THR:OG1	2.29	0.48
17:q:24:LEU:HD11	17:q:35:ASP:HB2	1.94	0.48
25:b:609:CLA:H202	25:b:612:CLA:H18	1.95	0.48
19:a:85:THR:HG21	19:a:113:GLN:HB2	1.96	0.48
20:c:80:LEU:HD21	25:c:603:CLA:H2A	1.95	0.48
8:r:160:GLU:N	24:r:307:CHL:O1D	2.46	0.48
5:K:8:LEU:HD11	5:K:19:VAL:HG21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:256:MET:HA	18:B:263:THR:HG21	1.94	0.48
20:C:249:ARG:NH1	22:W:109:ASP:O	2.46	0.48
33:D:411:LMG:H182	33:D:411:LMG:H211	1.52	0.48
11:5:14:PRO:HD2	24:5:305:CHL:HBB1	1.95	0.48
18:b:12:VAL:HG21	18:b:22:VAL:HG21	1.96	0.48
25:b:604:CLA:C1C	25:b:613:CLA:HBB1	2.44	0.48
11:2:73:LEU:HD23	11:2:81:PHE:HZ	1.79	0.48
12:9:221:VAL:HG13	12:9:222:THR:HG23	1.96	0.48
17:N:186:GLN:O	17:N:190:THR:OG1	2.25	0.48
17:8:58:ARG:HA	17:8:61:MET:HE3	1.95	0.48
2:e:95:ILE:O	21:d:84:SER:OG	2.23	0.48
12:u:249:THR:HB	12:u:250:ARG:HH21	1.78	0.48
18:b:283:GLU:CD	18:b:287:ARG:HH21	2.22	0.48
25:c:610:CLA:H151	25:c:610:CLA:H112	1.54	0.48
35:d:403:PHO:H112	35:d:403:PHO:H71	1.60	0.48
6:L:23:LEU:HD22	30:D:407:LHG:H262	1.95	0.48
18:B:334:ASP:OD1	18:B:334:ASP:N	2.47	0.48
10:4:41:ALA:HB1	12:6:76:GLU:HG3	1.96	0.48
12:6:68:THR:N	26:6:302:0IE:O42	2.45	0.48
17:g:159:PRO:HA	17:g:162:PHE:HB3	1.95	0.48
12:u:112:ASP:OD1	12:u:113:LEU:N	2.47	0.48
25:p:307:CLA:H12	17:q:39:LEU:HD11	1.95	0.48
18:b:208:LEU:HD23	25:b:602:CLA:HAC2	1.96	0.48
33:d:411:LMG:H321	33:d:411:LMG:H291	1.48	0.48
8:R:193:GLU:OE1	8:R:196:ARG:NH2	2.38	0.48
16:T:52:LEU:HD11	30:D:407:LHG:H171	1.96	0.48
17:N:68:LEU:HD13	17:N:195:VAL:HG22	1.96	0.48
18:B:154:GLY:HA2	18:B:158:VAL:HG23	1.95	0.48
12:p:145:ILE:HG23	12:p:146:LEU:HD12	1.96	0.48
21:d:55:ILE:O	21:d:66:SER:HB3	2.14	0.48
25:r:305:CLA:C1C	28:r:317:NEX:H222	2.44	0.48
28:r:317:NEX:H401	28:r:317:NEX:H35	1.57	0.48
11:5:88:LYS:HA	24:5:311:CHL:HED2	1.96	0.48
12:6:76:GLU:HA	12:6:79:LYS:HE3	1.96	0.48
12:6:162:TYR:HB3	24:6:311:CHL:CMC	2.43	0.48
17:n:24:LEU:HD22	17:n:33:GLY:HA2	1.95	0.48
12:7:74:ASP:HB3	12:7:77:MET:HE2	1.95	0.48
2:E:75:VAL:HG13	2:E:76:PHE:H	1.79	0.47
6:L:15:ARG:NH1	32:b:618:SQD:O2	2.44	0.47
6:L:24:LEU:HD13	30:A:601:LHG:H151	1.96	0.47
28:1:303:NEX:H383	25:1:307:CLA:C2B	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:156:MET:SD	28:3:318:NEX:H32	2.54	0.47
12:9:93:MET:HG3	12:9:205:GLY:HA2	1.95	0.47
18:B:283:GLU:CD	18:B:287:ARG:HH21	2.21	0.47
20:C:80:LEU:HD21	25:C:603:CLA:H2A	1.96	0.47
3:h:26:TYR:CE2	8:r:83:ILE:HG12	2.49	0.47
9:f:14:THR:HG21	14:x:100:VAL:HG11	1.94	0.47
11:5:147:GLY:C	11:5:149:ALA:H	2.22	0.47
12:6:59:GLU:OE1	12:6:59:GLU:N	2.47	0.47
17:q:45:THR:HG22	17:q:49:ASN:HD21	1.79	0.47
18:b:242:ILE:HG23	18:b:462:PHE:HD2	1.79	0.47
19:a:253:GLY:O	19:a:257:ARG:HG2	2.14	0.47
13:s:156:LEU:HD11	13:s:272:ALA:HB1	1.95	0.47
12:7:117:VAL:O	12:7:118:TRP:HB3	2.13	0.47
2:E:98:ARG:NH2	3:H:59:SER:OG	2.47	0.47
11:2:131:ARG:NH2	24:2:313:CHL:O1D	2.48	0.47
28:2:304:NEX:H35	28:2:304:NEX:H401	1.57	0.47
13:S:97:GLU:OE1	13:S:97:GLU:N	2.46	0.47
21:D:113:PHE:O	21:D:117:HIS:ND1	2.39	0.47
11:5:61:MET:HG3	11:5:173:GLY:HA2	1.96	0.47
11:5:118:TRP:HZ2	24:6:317:CHL:HBD	1.79	0.47
21:d:152:VAL:HG21	21:d:279:LEU:HD13	1.96	0.47
33:d:411:LMG:H162	33:d:411:LMG:H191	1.52	0.47
3:H:61:VAL:HG21	14:X:79:LEU:HD22	1.97	0.47
6:L:14:ASN:OD1	6:L:14:ASN:N	2.38	0.47
8:R:107:ASP:OD1	8:R:118:SER:OG	2.26	0.47
10:1:136:PRO:HG3	28:1:303:NEX:H183	1.97	0.47
24:3:309:CHL:H3A	28:3:318:NEX:C31	2.44	0.47
17:G:168:LYS:HD3	25:G:316:CLA:HAA2	1.96	0.47
20:C:204:SER:CB	33:C:618:LMG:HC71	2.44	0.47
4:i:31:ASN:HB3	19:a:135:PHE:CZ	2.49	0.47
24:q:308:CHL:HBA1	28:s:401:NEX:H403	1.96	0.47
20:c:211:TRP:CD2	20:c:212:ILE:HG23	2.49	0.47
13:s:131:MET:SD	25:s:410:CLA:HAB	2.54	0.47
8:r:154:PRO:HB3	8:r:256:GLY:HA3	1.95	0.47
10:1:168:LYS:NZ	25:1:315:CLA:O1D	2.40	0.47
10:1:210:GLY:HA2	25:1:316:CLA:CAD	2.44	0.47
28:1:303:NEX:O24	24:1:309:CHL:HAA1	2.15	0.47
28:S:617:NEX:H15	28:S:617:NEX:H201	1.62	0.47
28:G:304:NEX:C22	25:G:308:CLA:NC	2.77	0.47
17:N:168:LYS:HD3	25:N:315:CLA:HBD	1.96	0.47
19:A:170:ASP:OD2	20:C:345:ARG:NH1	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:601:LHG:O3	30:A:601:LHG:O1	2.23	0.47
20:C:211:TRP:CD2	20:C:212:ILE:HG23	2.49	0.47
20:C:365:LEU:H	20:C:365:LEU:HD12	1.79	0.47
6:l:11:VAL:H	7:m:28:LYS:HZ1	1.62	0.47
28:4:303:NEX:C36	25:4:307:CLA:C4B	2.89	0.47
28:6:303:NEX:O24	24:6:309:CHL:HAA2	2.13	0.47
25:g:315:CLA:H2A	25:g:315:CLA:HED3	1.96	0.47
12:u:86:VAL:HG21	12:u:176:LEU:HD13	1.96	0.47
24:u:305:CHL:H3A	24:u:305:CHL:HBA1	1.57	0.47
18:b:348:ASP:OD1	18:b:349:LYS:N	2.47	0.47
19:a:131:TRP:CH2	25:c:605:CLA:HAA2	2.50	0.47
12:3:59:GLU:OE1	12:3:59:GLU:N	2.47	0.47
26:9:302:0IE:C14	24:9:305:CHL:HMC	2.44	0.47
30:9:318:LHG:H261	30:9:318:LHG:HC82	1.96	0.47
17:N:8:ARG:NH2	17:N:24:LEU:O	2.46	0.47
17:N:168:LYS:HD3	25:N:315:CLA:HAA2	1.95	0.47
18:B:12:VAL:HG21	18:B:22:VAL:HG21	1.96	0.47
18:B:372:ASP:N	18:B:376:ILE:O	2.39	0.47
25:B:604:CLA:C1C	25:B:613:CLA:HBB1	2.44	0.47
32:B:618:SQD:O2	6:l:15:ARG:NH1	2.43	0.47
19:A:85:THR:HG21	19:A:113:GLN:HB2	1.96	0.47
10:4:88:LYS:HD3	24:4:310:CHL:HED2	1.95	0.47
28:4:303:NEX:H222	25:4:307:CLA:CHC	2.43	0.47
28:6:303:NEX:H401	28:6:303:NEX:H35	1.75	0.47
17:n:63:GLY:O	17:n:67:CYS:N	2.40	0.47
17:q:58:ARG:HA	17:q:61:MET:HE3	1.96	0.47
17:q:128:GLU:OE1	17:q:131:ARG:NH1	2.43	0.47
30:a:601:LHG:O3	30:a:601:LHG:O1	2.23	0.47
8:r:117:TYR:OH	8:r:128:GLU:OE1	2.26	0.47
11:2:133:ASN:ND2	12:3:46:PRO:O	2.48	0.47
13:S:59:PHE:CE2	28:S:617:NEX:C3	2.96	0.47
17:G:181:PHE:HE2	24:G:306:CHL:H172	1.79	0.47
25:G:315:CLA:HED3	25:G:315:CLA:H2A	1.97	0.47
12:9:226:PRO:HA	12:9:229:ASN:HD22	1.79	0.47
28:9:319:NEX:H35	28:9:319:NEX:H401	1.57	0.47
17:N:21:PRO:HD2	17:N:24:LEU:HD13	1.96	0.47
17:Y:21:PRO:HD2	17:Y:24:LEU:HD12	1.96	0.47
18:B:339:GLY:N	18:B:431:GLU:OE1	2.44	0.47
20:C:190:PRO:HB2	20:C:223:GLY:HA2	1.97	0.47
12:6:184:PRO:O	29:6:301:0UR:O40	2.32	0.47
17:y:24:LEU:HD11	17:y:35:ASP:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:p:87:ILE:HG22	24:p:313:CHL:HMD2	1.97	0.47
35:a:606:PHO:H61	35:a:606:PHO:H2	1.54	0.47
8:r:47:TRP:CD2	8:r:67:PHE:HD1	2.32	0.47
8:R:83:ILE:HD13	18:B:132:ALA:HB2	1.96	0.47
10:1:28:PHE:O	10:1:31:ASP:HB2	2.15	0.47
30:1:318:LHG:H111	30:1:318:LHG:HC82	1.76	0.47
12:3:124:GLN:O	12:3:127:SER:OG	2.24	0.47
24:3:309:CHL:HBA1	28:3:318:NEX:H31	1.96	0.47
13:S:128:ARG:HD2	25:S:609:CLA:C4C	2.45	0.47
13:S:295:LEU:O	13:S:299:ILE:HG13	2.14	0.47
17:G:171:LYS:NZ	25:G:315:CLA:O1D	2.38	0.47
18:B:272:ARG:NH1	18:B:276:ASP:OD2	2.48	0.47
19:A:227:THR:OG1	19:A:231:GLU:OE2	2.29	0.47
19:A:269:ARG:HE	21:D:235:PHE:HB2	1.79	0.47
10:4:171:LYS:NZ	30:4:318:LHG:O5	2.48	0.47
17:n:108:VAL:HG23	24:n:308:CHL:C1D	2.45	0.47
17:y:17:GLU:O	17:q:133:SER:OG	2.32	0.47
17:y:55:ILE:HG22	24:y:313:CHL:HMD2	1.96	0.47
12:p:76:GLU:O	12:p:80:GLN:NE2	2.48	0.47
12:p:130:GLY:HA3	12:p:142:ALA:O	2.15	0.47
18:b:251:VAL:HG22	25:b:602:CLA:H61	1.97	0.47
20:c:257:GLU:OE1	20:c:435:ARG:NH1	2.41	0.47
8:r:107:ASP:OD1	8:r:118:SER:OG	2.25	0.47
24:r:306:CHL:HBC2	24:r:307:CHL:HHD	1.97	0.47
12:7:124:GLN:O	12:7:127:SER:OG	2.22	0.47
12:7:230:TRP:NE1	24:7:318:CHL:HMC	2.27	0.47
24:7:305:CHL:H51	24:7:305:CHL:H12	1.68	0.47
8:R:56:TRP:NE1	8:R:68:ASP:OD2	2.45	0.47
13:S:286:HIS:CD2	13:S:290:PRO:HA	2.50	0.47
18:B:70:GLY:HA2	18:B:178:VAL:HG21	1.97	0.47
18:B:458:PHE:CE2	25:B:604:CLA:HAB	2.50	0.47
20:C:175:ASP:OD2	20:C:185:ARG:NH2	2.40	0.47
20:C:267:ILE:HD13	25:C:609:CLA:HED2	1.97	0.47
12:u:64:TYR:CE2	24:u:305:CHL:HHD	2.50	0.47
25:u:315:CLA:H41	25:u:315:CLA:H61	1.51	0.47
12:p:117:VAL:O	12:p:118:TRP:HB3	2.14	0.47
17:q:52:LEU:O	17:q:56:HIS:ND1	2.35	0.47
19:a:105:TRP:O	19:a:106:LEU:C	2.57	0.47
21:d:148:ALA:HB1	21:d:279:LEU:HB2	1.97	0.47
8:r:243:PHE:CD2	27:r:316:XAT:H12	2.50	0.47
11:2:120:GLN:HE21	24:2:313:CHL:HMC	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:304:NEX:H15	28:2:304:NEX:H201	1.62	0.47
12:9:112:ASP:OD1	12:9:113:LEU:N	2.48	0.47
12:9:147:ALA:HB1	24:9:308:CHL:HBC3	1.97	0.47
17:8:15:TYR:O	12:7:165:SER:OG	2.33	0.47
25:C:609:CLA:H112	25:C:609:CLA:H142	1.63	0.47
21:D:199:MET:HE3	21:D:281:MET:HB3	1.96	0.47
11:5:55:ILE:HG22	24:5:313:CHL:HMD2	1.97	0.47
12:u:52:VAL:HG12	12:u:65:GLY:HA3	1.97	0.47
25:d:405:CLA:HBA1	25:d:405:CLA:H3A	1.74	0.47
25:r:305:CLA:CMB	24:r:306:CHL:HBB1	2.45	0.47
28:7:304:NEX:H392	25:7:308:CLA:HMB2	1.97	0.47
24:7:305:CHL:H3A	24:7:305:CHL:HBA1	1.75	0.47
10:1:155:MET:N	10:1:155:MET:SD	2.88	0.47
12:3:162:TYR:HB3	24:3:311:CHL:CMC	2.45	0.47
13:S:58:TRP:C	13:S:60:GLY:H	2.23	0.47
13:S:129:TRP:O	13:S:133:GLY:N	2.41	0.47
24:9:304:CHL:HMD1	30:9:318:LHG:H251	1.96	0.47
18:B:251:VAL:HG22	25:B:602:CLA:H61	1.96	0.47
19:A:301:ASN:HB3	20:C:394:SER:HB2	1.96	0.47
3:h:13:THR:HG23	3:h:16:GLY:H	1.80	0.47
10:4:15:TYR:HD2	12:6:165:SER:HB2	1.79	0.47
28:4:303:NEX:C36	25:4:307:CLA:CHC	2.92	0.47
18:b:154:GLY:HA3	18:b:202:HIS:HB2	1.96	0.47
18:b:334:ASP:OD1	18:b:334:ASP:N	2.47	0.47
25:s:417:CLA:H3A	25:s:417:CLA:HBA2	1.59	0.47
4:I:31:ASN:HB3	19:A:135:PHE:CZ	2.49	0.46
6:L:11:VAL:H	7:M:28:LYS:HZ3	1.63	0.46
8:R:47:TRP:HE3	24:R:601:CHL:HAA1	1.79	0.46
10:1:14:PRO:HD2	24:1:304:CHL:HBB1	1.96	0.46
17:G:51:GLU:HG2	24:G:313:CHL:HED2	1.95	0.46
24:G:306:CHL:H93	25:G:307:CLA:HHB	1.96	0.46
24:G:313:CHL:HHC	24:G:313:CHL:HBB1	1.97	0.46
12:9:52:VAL:HG12	12:9:65:GLY:HA3	1.97	0.46
12:9:97:VAL:HG22	25:9:307:CLA:HMC1	1.97	0.46
28:N:303:NEX:H11	28:N:303:NEX:H191	1.80	0.46
19:A:38:LEU:HB3	19:A:39:PRO:HD3	1.97	0.46
17:g:17:GLU:OE1	17:g:17:GLU:N	2.46	0.46
17:y:9:ALA:HB1	24:y:305:CHL:HBC1	1.96	0.46
17:y:114:LEU:HD21	12:p:241:ASN:HD22	1.80	0.46
24:p:305:CHL:H121	24:p:305:CHL:H162	1.46	0.46
18:b:458:PHE:CE2	25:b:604:CLA:HAB	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:83:LEU:HD13	25:c:602:CLA:H143	1.96	0.46
13:s:131:MET:HG3	13:s:258:GLY:HA2	1.97	0.46
10:1:8:ARG:NH1	10:1:26:GLY:H	2.13	0.46
10:1:12:LEU:HA	24:1:304:CHL:NB	2.30	0.46
12:9:162:TYR:HB3	24:9:311:CHL:CMC	2.45	0.46
17:N:178:PHE:CE2	25:N:316:CLA:HAB	2.51	0.46
25:B:603:CLA:H61	25:B:603:CLA:H41	1.67	0.46
20:C:408:VAL:H	37:C:619:DGD:HE3	1.79	0.46
2:e:52:HIS:NE2	23:f:201:HEM:ND	2.63	0.46
17:g:49:ASN:ND2	24:g:306:CHL:H3A	2.31	0.46
12:u:162:TYR:HB3	24:u:312:CHL:CMC	2.45	0.46
17:n:178:PHE:CE2	25:n:316:CLA:HAB	2.50	0.46
28:n:303:NEX:H403	24:n:309:CHL:HBA2	1.98	0.46
19:a:28:LEU:HD11	21:d:258:GLY:HA2	1.97	0.46
21:d:242:GLU:OE1	21:d:264:LYS:NZ	2.32	0.46
7:M:28:LYS:HB2	7:m:27:VAL:HG12	1.97	0.46
17:G:164:GLU:O	17:G:167:THR:OG1	2.29	0.46
17:8:7:ASP:OD1	17:8:7:ASP:N	2.48	0.46
18:B:348:ASP:OD1	18:B:349:LYS:N	2.47	0.46
19:A:234:ASN:ND2	30:A:601:LHG:O4	2.48	0.46
28:u:304:NEX:C32	24:u:312:CHL:HMA1	2.46	0.46
24:y:305:CHL:HMA3	30:y:319:LHG:H112	1.97	0.46
17:q:142:ASP:OD1	17:q:145:TYR:N	2.40	0.46
18:b:8:VAL:HG23	18:b:9:HIS:CD2	2.49	0.46
20:c:190:PRO:HB2	20:c:223:GLY:HA2	1.97	0.46
8:r:69:PRO:O	27:r:316:XAT:O23	2.32	0.46
12:7:133:TYR:HH	28:7:304:NEX:H1	1.61	0.46
24:7:305:CHL:H162	24:7:305:CHL:H121	1.47	0.46
8:R:168:SER:HA	8:R:173:GLY:HA2	1.98	0.46
11:2:61:MET:HG3	11:2:173:GLY:HA2	1.96	0.46
28:2:304:NEX:H11	28:2:304:NEX:H191	1.82	0.46
17:8:39:LEU:HD11	25:7:307:CLA:H12	1.96	0.46
18:B:453:PHE:HB2	21:D:291:LEU:HD12	1.98	0.46
20:C:395:VAL:HG11	20:C:404:ALA:H	1.81	0.46
10:4:57:ALA:HB1	10:4:173:GLY:HA3	1.97	0.46
10:4:131:ARG:HG3	24:4:311:CHL:C1D	2.46	0.46
28:6:303:NEX:C28	24:6:309:CHL:CAA	2.89	0.46
28:y:304:NEX:H35	28:y:304:NEX:H401	1.58	0.46
22:w:103:GLN:OE1	20:c:250:ARG:NH1	2.48	0.46
18:b:346:PHE:HB2	18:b:354:LEU:O	2.16	0.46
18:b:426:LEU:HD13	18:b:443:PHE:HZ	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:604:CLA:H141	25:c:604:CLA:H192	1.98	0.46
21:d:51:GLY:HA3	21:d:78:VAL:HG22	1.97	0.46
8:R:162:ILE:HD11	25:R:604:CLA:H2A	1.97	0.46
11:2:8:ARG:NH1	11:2:31:ASP:O	2.36	0.46
28:3:318:NEX:H11	28:3:318:NEX:H191	1.80	0.46
13:S:58:TRP:CG	17:8:136:PRO:HG3	2.50	0.46
17:N:54:LEU:HD23	17:N:55:ILE:HD13	1.98	0.46
17:8:12:LEU:HD12	17:8:16:SER:HA	1.98	0.46
17:8:17:GLU:O	12:7:165:SER:OG	2.21	0.46
18:B:151:PHE:O	18:B:152:GLY:C	2.55	0.46
25:B:611:CLA:H112	25:B:611:CLA:H72	1.73	0.46
17:g:51:GLU:HG2	24:g:313:CHL:HED2	1.98	0.46
22:w:110:GLU:OE2	20:c:243:LYS:NZ	2.47	0.46
25:b:604:CLA:H71	25:b:604:CLA:H112	1.59	0.46
19:a:37:ARG:HH11	19:a:41:LEU:HD12	1.79	0.46
20:c:257:GLU:OE2	20:c:432:HIS:ND1	2.36	0.46
2:E:79:PRO:HD2	21:D:56:THR:HG21	1.98	0.46
2:E:106:LYS:HA	21:D:103:ARG:HH21	1.80	0.46
17:Y:194:PRO:O	29:Y:301:0UR:O39	2.33	0.46
25:A:603:CLA:HBD	25:A:604:CLA:HAC2	1.98	0.46
33:C:618:LMG:H172	33:C:618:LMG:H142	1.55	0.46
35:D:403:PHO:H112	35:D:403:PHO:H71	1.60	0.46
28:g:304:NEX:H15	28:g:304:NEX:H201	1.62	0.46
12:u:147:ALA:HB1	24:u:309:CHL:HBC3	1.96	0.46
24:y:313:CHL:HAA2	12:p:68:THR:HG21	1.98	0.46
25:a:603:CLA:HBD	25:a:604:CLA:HAC2	1.98	0.46
13:s:286:HIS:CD2	13:s:290:PRO:HA	2.50	0.46
8:r:44:ASP:CG	8:r:53:ARG:HH22	2.23	0.46
12:7:76:GLU:O	12:7:79:LYS:HG3	2.16	0.46
12:7:87:ILE:HG22	24:7:313:CHL:HMD2	1.97	0.46
24:3:309:CHL:H3A	28:3:318:NEX:C29	2.45	0.46
13:S:141:GLU:CD	13:S:280:TYR:HB3	2.41	0.46
18:B:60:MET:HB3	18:B:60:MET:HE2	1.64	0.46
18:B:208:LEU:HD23	25:B:602:CLA:HAC2	1.97	0.46
25:A:603:CLA:H203	30:D:407:LHG:H162	1.97	0.46
20:C:250:ARG:NH1	22:W:103:GLN:OE1	2.48	0.46
25:D:405:CLA:H161	25:D:405:CLA:H202	1.67	0.46
6:l:23:LEU:HD22	30:d:407:LHG:H262	1.96	0.46
28:6:303:NEX:H28	24:6:309:CHL:HAA1	1.97	0.46
17:g:61:MET:SD	25:g:314:CLA:HAB	2.56	0.46
17:g:200:GLU:O	17:g:208:ASN:ND2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:80:GLN:NE2	17:n:37:ALA:O	2.49	0.46
25:b:611:CLA:H112	25:b:611:CLA:H72	1.74	0.46
25:c:612:CLA:H43	24:s:402:CHL:HBB2	1.98	0.46
13:s:129:TRP:CE2	24:s:408:CHL:HED2	2.51	0.46
12:7:130:GLY:HA3	12:7:142:ALA:O	2.16	0.46
12:7:146:LEU:HD12	12:7:146:LEU:H	1.80	0.46
8:R:69:PRO:CD	27:R:615:XAT:O23	2.64	0.46
10:1:131:ARG:HG3	24:1:311:CHL:C1D	2.45	0.46
17:G:61:MET:SD	25:G:314:CLA:HAB	2.55	0.46
17:Y:126:LEU:O	17:Y:130:TYR:N	2.40	0.46
17:8:30:GLY:O	17:8:174:ARG:NH2	2.41	0.46
25:B:606:CLA:H13	25:B:613:CLA:HBB2	1.98	0.46
24:g:313:CHL:H111	24:g:313:CHL:H91	1.75	0.46
12:p:133:TYR:HE1	28:p:304:NEX:H1	1.50	0.46
8:r:193:GLU:OE1	8:r:196:ARG:NH2	2.37	0.46
8:R:44:ASP:HB2	8:R:53:ARG:HH22	1.81	0.46
28:R:616:NEX:H201	28:R:616:NEX:H15	1.62	0.46
13:S:127:CYS:HB3	13:S:258:GLY:HA3	1.98	0.46
13:S:156:LEU:HD11	13:S:272:ALA:HB1	1.97	0.46
25:G:315:CLA:H112	25:G:315:CLA:H72	1.82	0.46
12:9:80:GLN:NE2	17:N:37:ALA:O	2.49	0.46
17:N:59:TRP:CE2	24:N:311:CHL:HED2	2.51	0.46
18:B:23:HIS:O	18:B:27:THR:OG1	2.30	0.46
18:B:157:HIS:HE1	25:B:607:CLA:NA	2.14	0.46
18:B:326:ARG:HH21	21:D:297:ASP:CG	2.24	0.46
19:A:143:ILE:HD12	21:D:252:PHE:HE2	1.76	0.46
25:A:604:CLA:CHA	25:A:604:CLA:HBA1	2.46	0.46
25:C:604:CLA:H192	25:C:604:CLA:H141	1.98	0.46
10:4:155:MET:N	10:4:155:MET:SD	2.89	0.46
12:u:93:MET:HG3	12:u:205:GLY:HA2	1.98	0.46
22:w:76:ALA:H	20:c:202:LEU:HB3	1.81	0.46
19:a:105:TRP:O	19:a:107:TYR:N	2.48	0.46
2:E:104:GLN:O	2:E:107:SER:OG	2.26	0.46
4:I:28:PRO:O	4:I:31:ASN:ND2	2.48	0.46
10:1:74:GLU:HB3	10:1:81:PHE:HD2	1.81	0.46
17:Y:94:PHE:HZ	12:7:243:PHE:HB3	1.81	0.46
17:8:61:MET:SD	25:8:311:CLA:HAB	2.55	0.46
24:8:310:CHL:HBB1	24:8:310:CHL:HHC	1.98	0.46
25:B:613:CLA:H41	25:B:613:CLA:H62	1.53	0.46
21:D:186:GLN:OE1	21:D:192:THR:OG1	2.22	0.46
2:e:106:LYS:HA	21:d:103:ARG:HH21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:304:NEX:H11	28:u:304:NEX:H191	1.82	0.46
28:p:304:NEX:H15	28:p:304:NEX:H201	1.62	0.46
28:p:304:NEX:H35	28:p:304:NEX:H401	1.57	0.46
24:p:306:CHL:H91	24:p:306:CHL:H111	1.72	0.46
18:b:315:ILE:HG22	18:b:426:LEU:HB3	1.98	0.46
20:c:118:VAL:HG21	25:c:611:CLA:H152	1.97	0.46
21:d:186:GLN:OE1	21:d:192:THR:OG1	2.22	0.46
13:s:69:ASP:OD1	13:s:69:ASP:N	2.48	0.46
8:r:244:LEU:O	8:r:248:VAL:HG22	2.16	0.46
8:R:90:ALA:O	19:A:228:THR:OG1	2.23	0.45
11:2:21:PRO:HG2	11:2:35:ASP:HB3	1.99	0.45
13:S:68:LEU:HD21	13:S:249:GLU:HB3	1.98	0.45
24:G:305:CHL:H51	24:G:305:CHL:H12	1.76	0.45
25:Y:316:CLA:H2	25:Y:316:CLA:H61	1.59	0.45
11:5:73:LEU:HD23	11:5:81:PHE:HZ	1.80	0.45
24:6:304:CHL:H3A	24:6:304:CHL:HBA1	1.45	0.45
24:p:306:CHL:H143	24:p:306:CHL:H112	1.66	0.45
18:b:453:PHE:HB2	21:d:291:LEU:HD12	1.98	0.45
25:b:606:CLA:H13	25:b:613:CLA:HBB2	1.98	0.45
20:c:147:THR:O	20:c:151:ILE:HG13	2.16	0.45
21:d:29:PHE:O	21:d:128:ARG:NH1	2.46	0.45
28:s:401:NEX:H11	28:s:401:NEX:H191	1.80	0.45
8:r:146:VAL:HG11	25:r:305:CLA:HAC2	1.97	0.45
2:E:60:PHE:CZ	9:F:35:THR:HG21	2.52	0.45
8:R:93:ASN:OD1	8:R:93:ASN:N	2.48	0.45
8:R:154:PRO:HB3	8:R:256:GLY:HA3	1.98	0.45
24:3:304:CHL:HBA1	24:3:304:CHL:H3A	1.47	0.45
24:S:606:CHL:HHC	24:S:606:CHL:HBB1	1.97	0.45
28:S:617:NEX:C38	25:8:306:CLA:C2B	2.91	0.45
17:G:211:PHE:HB3	17:N:94:PHE:CZ	2.49	0.45
28:G:304:NEX:H15	28:G:304:NEX:H201	1.62	0.45
18:B:157:HIS:CE1	25:B:607:CLA:NA	2.84	0.45
19:A:131:TRP:CH2	25:C:605:CLA:HAA2	2.50	0.45
20:C:147:THR:O	20:C:151:ILE:HG13	2.16	0.45
1:z:2:ILE:O	1:z:6:GLN:HG2	2.17	0.45
12:6:168:PRO:HG2	24:6:311:CHL:HBB2	1.97	0.45
28:6:303:NEX:H11	28:6:303:NEX:H191	1.80	0.45
24:g:313:CHL:H43	24:u:305:CHL:H2	1.97	0.45
17:n:92:GLN:NE2	25:n:307:CLA:O1D	2.48	0.45
17:q:12:LEU:HD12	17:q:16:SER:HA	1.98	0.45
17:q:30:GLY:O	17:q:174:ARG:NH2	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:w:96:TRP:CZ2	33:w:201:LMG:H112	2.51	0.45
25:b:613:CLA:H92	25:b:613:CLA:H61	1.81	0.45
12:7:195:SER:C	12:7:197:LEU:H	2.24	0.45
6:L:27:VAL:HG21	30:A:601:LHG:H192	1.98	0.45
13:S:131:MET:HG3	13:S:258:GLY:HA2	1.98	0.45
19:A:28:LEU:HD11	21:D:258:GLY:HA2	1.99	0.45
20:C:45:ALA:O	20:C:49:VAL:HG23	2.17	0.45
30:D:408:LHG:H112	30:D:408:LHG:HC81	1.77	0.45
11:5:118:TRP:HA	11:5:121:VAL:HG12	1.99	0.45
12:6:72:SER:HB2	12:6:78:PHE:HA	1.99	0.45
12:u:210:PHE:HE2	25:u:317:CLA:HAB	1.81	0.45
22:w:96:TRP:CH2	33:w:201:LMG:H112	2.52	0.45
19:a:143:ILE:HD12	21:d:252:PHE:HE2	1.78	0.45
25:c:604:CLA:CAA	37:c:618:DGD:HD61	2.47	0.45
13:s:127:CYS:HB3	13:s:258:GLY:HA3	1.97	0.45
12:7:163:ARG:HG3	24:7:312:CHL:C1D	2.46	0.45
12:3:200:LYS:HD3	25:3:315:CLA:HAA2	1.97	0.45
24:Y:311:CHL:C4A	24:Y:311:CHL:HBA2	2.47	0.45
17:8:142:ASP:OD1	17:8:145:TYR:N	2.38	0.45
19:A:151:VAL:O	19:A:155:THR:HG23	2.16	0.45
19:A:299:GLY:O	20:C:391:SER:OG	2.27	0.45
21:D:29:PHE:O	21:D:128:ARG:NH1	2.46	0.45
28:g:304:NEX:C36	25:g:308:CLA:CHC	2.94	0.45
12:u:166:GLY:HA2	24:u:312:CHL:HMC	1.97	0.45
17:y:132:CYS:HB3	12:p:51:ASP:OD2	2.16	0.45
19:a:151:VAL:O	19:a:155:THR:HG23	2.16	0.45
20:c:365:LEU:HD12	20:c:365:LEU:H	1.81	0.45
11:2:85:VAL:HG21	11:2:88:LYS:HE3	1.99	0.45
28:G:304:NEX:C36	25:G:308:CLA:HAB	2.46	0.45
28:G:304:NEX:H401	28:G:304:NEX:H35	1.58	0.45
24:G:305:CHL:H62	24:G:305:CHL:H102	1.82	0.45
20:C:104:VAL:HG11	31:C:613:8CT:C05	2.47	0.45
33:D:411:LMG:H141	33:D:411:LMG:H171	1.77	0.45
11:5:21:PRO:HG2	11:5:35:ASP:HB3	1.98	0.45
12:u:100:LEU:O	12:u:104:LEU:N	2.28	0.45
12:u:145:ILE:H	12:u:145:ILE:HD12	1.82	0.45
17:n:168:LYS:HD3	25:n:315:CLA:HBD	1.98	0.45
24:n:305:CHL:H93	25:n:306:CLA:HHB	1.99	0.45
17:y:162:PHE:CE2	17:y:166:LYS:HD2	2.52	0.45
25:y:315:CLA:H112	25:y:315:CLA:H72	1.58	0.45
25:b:614:CLA:H41	25:b:614:CLA:H61	1.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:401:LMG:H141	33:d:401:LMG:H111	1.64	0.45
12:7:90:ARG:NH1	24:7:312:CHL:OBD	2.38	0.45
8:R:53:ARG:NH1	8:R:64:ASP:OD2	2.50	0.45
30:1:318:LHG:H142	30:1:318:LHG:H172	1.91	0.45
13:S:129:TRP:CE2	24:S:607:CHL:HED2	2.52	0.45
17:Y:116:ILE:HG12	24:Y:308:CHL:HAC1	1.98	0.45
17:Y:211:PHE:HB3	17:8:94:PHE:HZ	1.81	0.45
18:B:333:GLY:O	18:B:439:SER:HB3	2.17	0.45
25:B:604:CLA:H71	25:B:604:CLA:H112	1.67	0.45
21:D:51:GLY:HA3	21:D:78:VAL:HG22	1.98	0.45
7:m:17:ILE:HB	7:m:18:PRO:HD3	1.99	0.45
28:5:304:NEX:H362	25:5:308:CLA:C3B	2.46	0.45
12:u:55:TYR:OH	12:u:67:ASP:OD2	2.22	0.45
12:u:129:GLY:O	12:u:143:GLN:NE2	2.45	0.45
25:u:315:CLA:H72	25:u:316:CLA:ND	2.32	0.45
28:n:303:NEX:H35	28:n:303:NEX:H401	1.76	0.45
25:y:307:CLA:H12	12:p:71:LEU:HD11	1.99	0.45
25:p:314:CLA:H43	25:p:316:CLA:HBA1	1.98	0.45
17:q:61:MET:SD	25:q:312:CLA:HAB	2.56	0.45
20:c:267:ILE:HD13	25:c:609:CLA:HED2	1.98	0.45
12:7:92:ALA:O	12:7:96:THR:HG22	2.17	0.45
28:2:304:NEX:H173	17:N:152:PRO:HB2	1.97	0.45
25:3:307:CLA:CBA	28:3:318:NEX:H241	2.47	0.45
24:3:309:CHL:HAA1	28:3:318:NEX:H381	1.98	0.45
17:G:162:PHE:CE2	17:G:166:LYS:HD2	2.51	0.45
18:B:346:PHE:HB2	18:B:354:LEU:O	2.17	0.45
25:B:609:CLA:H142	25:B:612:CLA:H72	1.99	0.45
25:C:601:CLA:H2A	25:C:601:CLA:O1D	2.16	0.45
21:D:55:ILE:O	21:D:66:SER:HB3	2.17	0.45
21:D:87:HIS:CD2	21:D:87:HIS:H	2.35	0.45
21:D:87:HIS:CE1	21:D:162:LEU:HA	2.51	0.45
4:i:9:TYR:HD2	22:w:88:LEU:HD11	1.82	0.45
7:m:3:VAL:HG22	33:m:101:LMG:O3	2.17	0.45
28:u:304:NEX:H15	28:u:304:NEX:H201	1.62	0.45
17:n:168:LYS:O	17:n:172:ASN:ND2	2.26	0.45
17:y:110:ALA:HA	24:y:309:CHL:CHC	2.47	0.45
17:y:126:LEU:O	17:y:130:TYR:N	2.40	0.45
28:y:304:NEX:H11	28:y:304:NEX:H191	1.82	0.45
28:p:304:NEX:H11	28:p:304:NEX:H191	1.82	0.45
18:b:153:PHE:O	18:b:158:VAL:HG23	2.17	0.45
25:b:602:CLA:H11	25:b:602:CLA:H52	1.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:227:THR:OG1	19:a:228:THR:N	2.50	0.45
20:c:59:GLU:O	20:c:63:PHE:HB2	2.17	0.45
20:c:408:VAL:H	37:c:618:DGD:HE3	1.79	0.45
25:c:601:CLA:H2A	25:c:601:CLA:O1D	2.16	0.45
30:d:408:LHG:H112	30:d:408:LHG:HC81	1.40	0.45
24:r:303:CHL:HBB2	27:r:316:XAT:H32	1.98	0.45
12:7:133:TYR:HE1	28:7:304:NEX:H241	1.81	0.45
12:7:174:ASP:OD1	12:7:176:LEU:N	2.42	0.45
28:7:304:NEX:C32	24:7:310:CHL:HBA1	2.43	0.45
35:A:606:PHO:H141	35:A:606:PHO:H161	1.69	0.45
20:C:151:ILE:HD13	25:C:616:CLA:HAB	1.99	0.45
12:6:143:GLN:N	24:6:308:CHL:OMC	2.44	0.45
24:y:305:CHL:HBA1	24:y:305:CHL:H3A	1.64	0.45
12:p:195:SER:C	12:p:197:LEU:H	2.23	0.45
18:b:70:GLY:HA2	18:b:178:VAL:HG21	1.98	0.45
20:c:228:ILE:H	20:c:228:ILE:HG12	1.63	0.45
8:r:65:ARG:NH2	8:r:230:GLU:OE2	2.50	0.45
12:7:91:TRP:CE2	24:7:312:CHL:HED2	2.52	0.45
8:R:135:ARG:HD2	24:R:607:CHL:OBD	2.17	0.45
24:3:309:CHL:CAA	28:3:318:NEX:C28	2.92	0.45
13:S:69:ASP:OD1	13:S:69:ASP:N	2.49	0.45
12:9:98:GLY:H	12:9:101:THR:HG23	1.82	0.45
24:Y:304:CHL:HHB	24:8:310:CHL:HMB3	1.99	0.45
25:B:606:CLA:H102	25:B:606:CLA:H61	1.67	0.45
20:C:59:GLU:O	20:C:63:PHE:HB2	2.16	0.45
33:m:101:LMG:O4	18:b:328:GLY:HA3	2.17	0.45
11:5:123:ILE:HG23	28:5:304:NEX:C15	2.46	0.45
28:6:303:NEX:H31	24:6:309:CHL:HBA2	1.99	0.45
28:n:303:NEX:H15	28:n:303:NEX:H201	1.86	0.45
17:y:158:ASP:HB3	17:y:161:THR:HG22	1.99	0.45
24:y:306:CHL:H142	24:y:306:CHL:H112	1.67	0.45
12:p:174:ASP:OD1	12:p:176:LEU:N	2.43	0.45
18:b:326:ARG:HH21	21:d:297:ASP:CG	2.24	0.45
25:c:612:CLA:OBD	13:s:81:PRO:HB2	2.17	0.45
35:d:403:PHO:H41	35:d:403:PHO:H61	1.45	0.45
13:s:232:GLY:HA2	13:s:236:ASP:HB2	1.99	0.45
24:7:306:CHL:H111	24:7:306:CHL:H91	1.77	0.45
28:2:304:NEX:H362	25:2:308:CLA:C3B	2.47	0.45
28:G:304:NEX:H11	28:G:304:NEX:H191	1.82	0.45
25:G:314:CLA:H43	25:G:316:CLA:HBA1	1.98	0.45
17:N:110:ALA:O	17:N:111:GLN:NE2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:278:TRP:HB3	19:A:279:PRO:HD3	1.98	0.45
33:C:618:LMG:H331	33:C:618:LMG:H362	1.48	0.45
6:l:27:VAL:HG21	30:a:601:LHG:H192	1.98	0.45
10:4:12:LEU:HA	24:4:304:CHL:NB	2.32	0.45
11:5:85:VAL:HG21	11:5:88:LYS:HE3	1.99	0.45
12:6:91:TRP:CE2	24:6:311:CHL:HED2	2.51	0.45
17:g:110:ALA:HA	24:g:309:CHL:CHC	2.47	0.45
28:g:304:NEX:C28	24:g:310:CHL:HAA1	2.47	0.45
12:u:212:MET:HE2	12:u:212:MET:HB2	1.85	0.45
17:n:137:LEU:HG	24:n:311:CHL:HBB1	1.99	0.45
17:y:189:GLN:OE1	26:y:303:0IE:O40	2.35	0.45
28:p:304:NEX:C38	25:p:308:CLA:CHB	2.93	0.45
18:b:132:ALA:HB2	8:r:83:ILE:HD13	1.99	0.45
19:a:278:TRP:HB3	19:a:279:PRO:HD3	1.98	0.45
21:d:110:LEU:HD12	21:d:110:LEU:HA	1.77	0.45
28:7:304:NEX:C38	25:7:308:CLA:C1B	2.84	0.45
8:R:41:LYS:O	8:R:43:SER:N	2.50	0.44
10:1:13:GLY:O	10:1:16:SER:OG	2.35	0.44
17:G:17:GLU:OE1	17:G:17:GLU:N	2.47	0.44
28:G:304:NEX:H15	24:G:312:CHL:HMB3	1.98	0.44
12:9:91:TRP:CD1	24:9:312:CHL:HMD3	2.51	0.44
28:N:303:NEX:H35	28:N:303:NEX:H401	1.75	0.44
18:B:61:PHE:HE1	18:B:451:PHE:HB2	1.82	0.44
25:C:604:CLA:HAA2	37:C:619:DGD:HD61	1.99	0.44
35:D:403:PHO:H72	25:D:404:CLA:H111	1.99	0.44
17:g:168:LYS:HD3	25:g:316:CLA:HAA2	1.97	0.44
17:n:54:LEU:HD23	17:n:55:ILE:HD13	1.98	0.44
18:b:462:PHE:HA	25:b:611:CLA:HMC1	1.99	0.44
19:a:38:LEU:HB3	19:a:39:PRO:HD3	1.99	0.44
13:s:58:TRP:C	13:s:60:GLY:N	2.75	0.44
13:s:175:TRP:HE1	25:s:417:CLA:C4B	2.30	0.44
8:R:156:GLN:H	8:R:156:GLN:HG3	1.40	0.44
24:G:306:CHL:H92	24:G:306:CHL:H62	1.70	0.44
25:9:307:CLA:H42	24:9:309:CHL:HBD	1.98	0.44
5:k:23:PRO:O	5:k:26:PRO:HD2	2.17	0.44
12:6:57:THR:OG1	12:6:59:GLU:OE1	2.24	0.44
17:n:54:LEU:HD21	17:n:58:ARG:CZ	2.46	0.44
25:r:313:CLA:HBA2	25:r:313:CLA:H3A	1.61	0.44
12:7:162:TYR:HB3	24:7:312:CHL:CMC	2.47	0.44
28:R:616:NEX:H35	28:R:616:NEX:H401	1.58	0.44
28:1:303:NEX:H401	28:1:303:NEX:H35	1.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:191:PRO:HA	12:3:194:PHE:HB3	1.99	0.44
25:G:317:CLA:H61	25:G:317:CLA:H2	1.73	0.44
12:9:91:TRP:O	12:9:95:GLY:N	2.51	0.44
18:B:315:ILE:HG22	18:B:426:LEU:HB3	1.98	0.44
25:B:605:CLA:HBC3	25:B:606:CLA:H42	1.99	0.44
33:B:619:LMG:H161	33:B:619:LMG:H132	1.58	0.44
12:u:158:LEU:CD2	28:u:304:NEX:H203	2.26	0.44
28:u:304:NEX:H401	28:u:304:NEX:H35	1.58	0.44
25:b:613:CLA:H143	25:b:613:CLA:H111	1.75	0.44
25:b:615:CLA:H8	25:b:616:CLA:HBB1	1.99	0.44
20:c:178:ALA:HB3	20:c:182:GLY:HA2	1.99	0.44
8:r:135:ARG:HD2	24:r:308:CHL:OBD	2.17	0.44
8:R:128:GLU:O	8:R:132:ILE:HG12	2.18	0.44
25:R:604:CLA:HMB1	24:R:605:CHL:HBB1	2.00	0.44
11:2:106:GLU:CD	11:2:106:GLU:H	2.26	0.44
13:S:175:TRP:HE1	25:S:616:CLA:C4B	2.30	0.44
12:9:53:PRO:HG3	12:9:67:ASP:HB3	1.99	0.44
24:9:305:CHL:HBB1	24:9:305:CHL:H51	1.99	0.44
25:9:316:CLA:H11	25:9:316:CLA:C4D	2.48	0.44
25:N:306:CLA:HAC1	24:N:310:CHL:HBB2	2.00	0.44
25:A:603:CLA:HBB1	25:A:603:CLA:HMB3	2.00	0.44
25:C:604:CLA:H71	37:C:619:DGD:HBT1	1.99	0.44
3:h:66:ILE:HD11	18:b:187:ALA:O	2.18	0.44
17:g:93:ILE:HG12	17:g:113:ILE:HB	1.99	0.44
17:n:24:LEU:HD12	17:n:24:LEU:H	1.81	0.44
17:n:59:TRP:CE2	24:n:311:CHL:HED2	2.52	0.44
17:y:194:PRO:O	29:y:301:0UR:O39	2.35	0.44
12:p:92:ALA:O	12:p:96:THR:HG22	2.18	0.44
25:b:601:CLA:HBB1	25:b:602:CLA:CHC	2.47	0.44
21:d:236:ASN:HB3	21:d:239:GLN:HB3	2.00	0.44
13:s:174:PRO:HG3	25:s:417:CLA:NA	2.33	0.44
8:R:160:GLU:N	24:R:606:CHL:O1D	2.49	0.44
28:1:303:NEX:H362	25:1:307:CLA:CAB	2.48	0.44
12:3:133:TYR:HE1	28:3:318:NEX:H1	1.64	0.44
13:S:162:MET:O	13:S:163:LEU:C	2.60	0.44
13:S:188:ALA:O	13:S:192:VAL:HG23	2.17	0.44
25:9:307:CLA:HBA2	25:9:307:CLA:H3A	1.57	0.44
17:Y:147:GLY:C	17:Y:149:ALA:H	2.26	0.44
18:B:53:ASN:ND2	18:B:53:ASN:O	2.50	0.44
25:B:612:CLA:H141	25:B:612:CLA:H161	1.75	0.44
25:B:615:CLA:H8	25:B:616:CLA:HBB1	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:203:GLY:HA3	21:D:278:GLY:HA3	1.99	0.44
24:n:305:CHL:H92	24:n:305:CHL:H62	1.72	0.44
25:b:609:CLA:H193	25:b:612:CLA:H141	1.98	0.44
13:s:198:ALA:HA	13:s:201:TYR:CD2	2.53	0.44
8:r:48:MET:HE3	8:r:48:MET:HB2	1.81	0.44
7:M:17:ILE:HB	7:M:18:PRO:HD3	1.98	0.44
12:3:91:TRP:CE2	24:3:311:CHL:HED2	2.53	0.44
12:9:86:VAL:HG21	12:9:176:LEU:HD13	1.99	0.44
12:9:117:VAL:HG23	12:9:118:TRP:H	1.83	0.44
12:9:145:ILE:H	12:9:145:ILE:HD12	1.82	0.44
17:Y:120:GLN:OE1	24:Y:310:CHL:HMC	2.17	0.44
17:8:40:SER:OG	24:8:304:CHL:HAA2	2.17	0.44
17:8:147:GLY:C	17:8:149:ALA:H	2.25	0.44
19:A:281:VAL:HG13	32:A:609:SQD:H182	1.98	0.44
25:C:607:CLA:H142	25:C:607:CLA:H111	1.82	0.44
10:4:10:LEU:HB2	10:4:16:SER:HB3	2.00	0.44
24:4:304:CHL:OBD	24:4:305:CHL:HHD	2.17	0.44
12:6:122:GLY:HA2	24:6:309:CHL:HAC2	1.99	0.44
17:n:186:GLN:O	17:n:190:THR:OG1	2.24	0.44
24:n:304:CHL:H3A	24:n:304:CHL:HBA1	1.69	0.44
25:n:306:CLA:HAC1	24:n:310:CHL:HBB2	2.00	0.44
12:p:80:GLN:H	12:p:80:GLN:HG2	1.45	0.44
12:p:100:LEU:O	12:p:104:LEU:N	2.29	0.44
17:q:147:GLY:C	17:q:149:ALA:H	2.25	0.44
18:b:333:GLY:O	18:b:439:SER:HB3	2.17	0.44
19:a:55:ALA:O	19:a:70:SER:OG	2.28	0.44
13:s:141:GLU:CD	13:s:280:TYR:HB3	2.41	0.44
28:s:401:NEX:H35	28:s:401:NEX:H401	1.76	0.44
25:s:413:CLA:H2	24:s:414:CHL:HMD1	1.98	0.44
12:7:186:ASN:OD1	12:7:186:ASN:N	2.50	0.44
10:1:134:GLY:HA2	24:1:311:CHL:HAC1	2.00	0.44
28:2:304:NEX:H163	17:N:153:MET:HG2	2.00	0.44
12:3:122:GLY:HA2	24:3:309:CHL:HAC2	1.98	0.44
13:S:231:PRO:HB3	24:S:607:CHL:HBC2	1.99	0.44
13:S:232:GLY:HA2	13:S:236:ASP:HB2	2.00	0.44
24:G:306:CHL:H143	24:G:306:CHL:H112	1.73	0.44
25:9:314:CLA:H61	25:9:314:CLA:H41	1.45	0.44
25:8:305:CLA:HED1	24:8:310:CHL:H92	2.00	0.44
25:B:614:CLA:H41	25:B:614:CLA:H61	1.47	0.44
19:A:68:SER:OG	19:A:69:GLY:N	2.51	0.44
35:A:606:PHO:H61	35:A:606:PHO:H2	1.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:610:CLA:O2A	25:C:610:CLA:H2A	2.18	0.44
1:z:41:PHE:CZ	13:s:84:LEU:HG	2.53	0.44
3:h:67:ALA:HB3	3:h:72:SER:HB3	1.99	0.44
11:5:120:GLN:HE21	24:5:313:CHL:HMC	1.82	0.44
28:6:303:NEX:H31	24:6:309:CHL:HBA1	2.00	0.44
24:n:304:CHL:ND	30:n:318:LHG:HC82	2.33	0.44
12:p:105:LEU:O	12:p:111:VAL:HG13	2.17	0.44
17:q:135:GLY:H	24:q:310:CHL:CMC	2.31	0.44
18:b:53:ASN:ND2	18:b:53:ASN:O	2.50	0.44
13:s:268:PHE:HD2	13:s:279:PRO:HG2	1.83	0.44
8:r:76:VAL:O	8:r:104:THR:OG1	2.36	0.44
12:7:180:GLU:C	12:7:182:PHE:H	2.25	0.44
5:K:40:VAL:HG11	5:K:43:ARG:CZ	2.48	0.44
13:S:81:PRO:HB2	25:C:612:CLA:OBD	2.18	0.44
13:S:198:ALA:HA	13:S:201:TYR:CD2	2.53	0.44
24:N:304:CHL:ND	30:N:318:LHG:HC82	2.32	0.44
24:Y:312:CHL:H92	24:Y:312:CHL:H62	1.70	0.44
17:8:12:LEU:HD23	24:8:303:CHL:HHB	1.99	0.44
18:B:63:LEU:HD12	18:B:66:MET:HE3	2.00	0.44
18:B:228:ALA:HA	33:D:411:LMG:HC71	1.99	0.44
25:B:604:CLA:H93	25:B:604:CLA:H61	1.77	0.44
20:C:210:GLY:HA3	20:C:214:SER:HB3	1.98	0.44
12:6:209:MET:HB2	24:6:305:CHL:HMC	2.00	0.44
12:u:84:LEU:O	12:u:88:HIS:ND1	2.48	0.44
17:y:120:GLN:OE1	24:y:311:CHL:HMC	2.17	0.44
24:y:305:CHL:HHB	24:q:311:CHL:HMB3	2.00	0.44
17:q:40:SER:OG	24:q:304:CHL:HAA2	2.18	0.44
22:w:75:ARG:H	22:w:75:ARG:HD2	1.83	0.44
20:c:45:ALA:O	20:c:49:VAL:HG23	2.17	0.44
25:c:604:CLA:H71	37:c:618:DGD:HBT1	1.99	0.44
21:d:199:MET:HE3	21:d:281:MET:HB3	1.99	0.44
1:Z:41:PHE:CZ	13:S:84:LEU:HG	2.53	0.44
3:H:13:THR:HG23	3:H:16:GLY:H	1.83	0.44
8:R:213:ASP:O	8:R:216:ASN:ND2	2.51	0.44
24:S:601:CHL:H3A	24:S:601:CHL:HBA1	1.56	0.44
28:S:617:NEX:H401	28:S:617:NEX:H35	1.57	0.44
17:G:104:ASN:HB3	17:G:107:LEU:HD23	1.98	0.44
25:B:612:CLA:H41	25:B:612:CLA:H61	1.44	0.44
20:C:385:THR:HG1	20:C:386:HIS:CE1	2.36	0.44
25:C:601:CLA:H143	25:C:601:CLA:H162	1.84	0.44
33:C:618:LMG:H151	33:C:618:LMG:H122	1.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:51:GLU:HG3	10:4:144:LEU:HD21	2.00	0.44
28:6:303:NEX:H28	24:6:309:CHL:CAA	2.48	0.44
25:6:316:CLA:H3A	25:6:316:CLA:HBA2	1.71	0.44
24:g:305:CHL:H12	24:g:305:CHL:H51	1.77	0.44
24:n:308:CHL:HAA2	25:r:313:CLA:H3A	2.00	0.44
25:q:306:CLA:C3B	28:s:401:NEX:H383	2.48	0.44
25:a:604:CLA:CHA	25:a:604:CLA:HBA1	2.46	0.44
20:c:151:ILE:HD13	25:c:616:CLA:HAB	2.00	0.44
13:s:199:GLU:HG2	24:s:409:CHL:CHB	2.48	0.44
1:Z:33:TRP:O	1:Z:37:LYS:HB2	2.18	0.43
2:E:73:TYR:CD1	2:E:80:ARG:HG2	2.53	0.43
8:R:244:LEU:O	8:R:248:VAL:HG22	2.16	0.43
11:2:147:GLY:C	11:2:149:ALA:H	2.24	0.43
17:G:59:TRP:CD1	24:G:313:CHL:HMD3	2.53	0.43
28:G:304:NEX:C15	24:G:312:CHL:HMB2	2.44	0.43
24:G:313:CHL:H91	24:G:313:CHL:H111	1.76	0.43
17:Y:132:CYS:HB3	12:7:51:ASP:OD2	2.17	0.43
25:B:601:CLA:HBB1	25:B:602:CLA:CHC	2.48	0.43
20:C:132:PHE:CE1	25:C:612:CLA:HAA1	2.53	0.43
20:C:285:TYR:O	20:C:411:ARG:NH2	2.50	0.43
35:D:403:PHO:H41	35:D:403:PHO:H61	1.44	0.43
11:5:12:LEU:HB2	11:5:16:SER:HB3	2.00	0.43
12:u:102:PRO:O	12:u:116:PRO:HB2	2.18	0.43
12:u:218:GLN:O	12:u:222:THR:OG1	2.25	0.43
17:n:40:SER:HA	17:n:45:THR:HG23	2.00	0.43
17:y:211:PHE:HB3	17:q:94:PHE:HZ	1.82	0.43
25:b:606:CLA:H61	25:b:606:CLA:H102	1.62	0.43
19:a:259:ILE:HD12	19:a:263:ALA:HB3	1.99	0.43
25:d:405:CLA:H143	25:d:405:CLA:H161	1.78	0.43
28:r:317:NEX:H11	28:r:317:NEX:H191	1.82	0.43
25:7:314:CLA:H43	25:7:316:CLA:HBA1	2.00	0.43
3:H:58:ASN:C	3:H:59:SER:HG	2.25	0.43
10:1:54:LEU:HD23	10:1:144:LEU:HB3	1.99	0.43
11:2:59:TRP:CE2	24:2:312:CHL:HED2	2.53	0.43
25:2:315:CLA:H111	25:2:315:CLA:H72	1.72	0.43
12:3:213:PHE:HD1	25:3:306:CLA:HBB2	1.82	0.43
17:G:49:ASN:ND2	24:G:306:CHL:H3A	2.34	0.43
21:D:242:GLU:OE1	21:D:264:LYS:NZ	2.32	0.43
17:g:162:PHE:CE2	17:g:166:LYS:HD2	2.53	0.43
24:g:305:CHL:H62	24:g:305:CHL:H102	1.82	0.43
12:u:45:GLY:O	12:u:48:SER:OG	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:165:SER:OG	17:n:15:TYR:O	2.30	0.43
17:q:136:PRO:HG3	13:s:58:TRP:CG	2.53	0.43
17:q:168:LYS:HD3	25:q:314:CLA:HAA2	2.00	0.43
24:q:303:CHL:H41	24:q:303:CHL:H61	1.61	0.43
20:c:104:VAL:HG11	31:c:613:8CT:C05	2.48	0.43
25:c:610:CLA:O2A	25:c:610:CLA:H2A	2.18	0.43
13:s:188:ALA:O	13:s:192:VAL:HG23	2.18	0.43
30:7:319:LHG:H242	30:7:319:LHG:H272	1.71	0.43
30:9:318:LHG:H122	30:9:318:LHG:HC91	1.82	0.43
17:N:134:GLY:HA2	24:N:311:CHL:HAC1	1.98	0.43
17:8:53:GLU:HB2	24:8:304:CHL:CHB	2.48	0.43
20:C:83:LEU:HD13	25:C:602:CLA:H143	2.00	0.43
20:C:151:ILE:HG21	25:C:616:CLA:C3B	2.48	0.43
21:D:148:ALA:HB1	21:D:279:LEU:HB2	2.00	0.43
1:z:33:TRP:O	1:z:37:LYS:HB2	2.18	0.43
28:4:303:NEX:H221	25:4:307:CLA:C1C	2.48	0.43
24:g:318:CHL:HBD	17:n:118:TRP:HE1	1.83	0.43
12:u:147:ALA:HB3	24:u:309:CHL:HMC	2.00	0.43
25:n:316:CLA:H3A	25:n:316:CLA:HBA2	1.81	0.43
17:y:15:TYR:O	17:q:133:SER:OG	2.24	0.43
18:b:61:PHE:HE1	18:b:451:PHE:HB2	1.81	0.43
19:a:68:SER:HB3	21:d:313:THR:HG22	2.01	0.43
35:a:606:PHO:H161	35:a:606:PHO:H141	1.70	0.43
13:s:58:TRP:NE1	28:s:401:NEX:C19	2.77	0.43
8:r:128:GLU:O	8:r:132:ILE:HG12	2.17	0.43
12:7:83:GLU:HA	12:7:176:LEU:HD11	2.00	0.43
26:7:302:0IE:C13	24:7:306:CHL:HMC	2.48	0.43
5:K:23:PRO:O	5:K:26:PRO:HD2	2.17	0.43
11:2:218:LYS:HE3	11:2:221:PHE:H	1.84	0.43
24:9:304:CHL:H3A	24:9:304:CHL:HBA1	1.62	0.43
17:N:147:GLY:C	17:N:149:ALA:H	2.27	0.43
19:A:114:LEU:O	19:A:118:HIS:ND1	2.46	0.43
20:C:431:TRP:HH2	30:D:408:LHG:HC62	1.84	0.43
33:m:101:LMG:H121	25:b:608:CLA:ND	2.33	0.43
11:5:106:GLU:CD	11:5:106:GLU:H	2.26	0.43
12:6:183:ASP:OD1	12:6:186:ASN:HA	2.17	0.43
17:g:101:TYR:CE2	28:g:304:NEX:O23	2.68	0.43
24:y:312:CHL:C4A	24:y:312:CHL:HBA2	2.47	0.43
12:p:113:LEU:HD21	12:p:134:LEU:HD23	2.00	0.43
12:p:162:TYR:HB3	24:p:312:CHL:CMC	2.46	0.43
12:p:195:SER:O	12:p:196:GLU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:63:LEU:HD12	18:b:66:MET:HE3	2.00	0.43
18:b:80:ILE:HD13	18:b:80:ILE:HA	1.89	0.43
19:a:225:ARG:HD2	19:a:225:ARG:N	2.33	0.43
19:a:246:TYR:CE2	19:a:248:ILE:HG12	2.54	0.43
20:c:132:PHE:CE1	25:c:612:CLA:HAA1	2.54	0.43
20:c:151:ILE:HG21	25:c:616:CLA:C3B	2.48	0.43
37:c:619:DGD:HB91	37:c:619:DGD:HB62	1.36	0.43
5:K:28:LEU:HB3	31:V:401:8CT:C18	2.49	0.43
11:2:54:LEU:HD23	11:2:144:LEU:HD22	2.00	0.43
13:S:174:PRO:HG3	25:S:616:CLA:NA	2.33	0.43
25:S:612:CLA:H2	24:S:613:CHL:HMD1	2.00	0.43
17:N:39:LEU:HD12	24:N:305:CHL:H11	1.99	0.43
24:N:304:CHL:H41	24:N:304:CHL:H61	1.74	0.43
17:Y:136:PRO:CG	28:r:301:NEX:H192	2.49	0.43
18:B:463:PHE:CE1	33:D:401:LMG:H421	2.54	0.43
25:A:604:CLA:H111	25:A:604:CLA:H151	1.89	0.43
20:C:178:ALA:HB3	20:C:182:GLY:HA2	2.01	0.43
20:C:439:ALA:HA	20:C:444:GLU:HB3	2.00	0.43
21:D:123:ILE:HD11	33:D:401:LMG:H392	2.00	0.43
25:5:315:CLA:H72	25:5:315:CLA:H111	1.73	0.43
17:n:178:PHE:HE2	25:n:316:CLA:HAB	1.83	0.43
17:y:188:LEU:HD12	17:y:218:PHE:HD2	1.84	0.43
12:p:216:PHE:O	12:p:220:ILE:HG13	2.18	0.43
18:b:433:ASP:OD1	18:b:433:ASP:N	2.48	0.43
19:a:10:GLY:HA3	19:a:15:GLU:CD	2.43	0.43
25:c:602:CLA:H92	25:c:602:CLA:H61	1.77	0.43
13:s:212:ALA:O	13:s:214:GLY:N	2.44	0.43
8:r:109:VAL:HG22	8:r:111:THR:HG22	2.01	0.43
8:r:179:SER:O	8:r:183:TRP:HD1	2.02	0.43
8:R:86:LEU:HG	8:R:88:GLN:HG2	2.00	0.43
11:2:55:ILE:HG22	24:2:313:CHL:HMD2	1.98	0.43
12:3:40:ARG:NE	12:3:63:ASP:O	2.28	0.43
13:S:124:LEU:O	13:S:128:ARG:HG2	2.18	0.43
17:G:174:ARG:HA	17:G:177:MET:HE2	2.00	0.43
12:9:77:MET:O	12:9:80:GLN:NE2	2.52	0.43
28:9:319:NEX:H11	28:9:319:NEX:H191	1.82	0.43
24:Y:304:CHL:H3A	24:Y:304:CHL:HBA1	1.65	0.43
18:B:435:ALA:O	18:B:436:THR:OG1	2.28	0.43
18:B:435:ALA:C	18:B:437:LEU:H	2.27	0.43
25:B:615:CLA:H2	25:B:616:CLA:CBB	2.39	0.43
19:A:225:ARG:HD2	19:A:225:ARG:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:263:ASN:HB3	21:D:266:TRP:HB3	1.99	0.43
10:4:168:LYS:O	10:4:172:ASN:ND2	2.25	0.43
12:6:170:GLY:HA3	24:6:311:CHL:HBC3	1.99	0.43
12:u:43:TRP:CG	12:u:66:TRP:HB2	2.54	0.43
25:u:307:CLA:H92	25:u:307:CLA:H61	1.79	0.43
17:n:147:GLY:C	17:n:149:ALA:H	2.27	0.43
18:b:92:SER:OG	18:b:93:TYR:N	2.51	0.43
25:b:603:CLA:H161	25:b:603:CLA:H143	1.72	0.43
25:b:605:CLA:HBC3	25:b:606:CLA:H42	2.01	0.43
13:s:162:MET:O	13:s:163:LEU:C	2.60	0.43
2:E:103:GLU:HA	2:E:106:LYS:HB2	2.00	0.43
8:R:243:PHE:CZ	27:R:615:XAT:H10	2.54	0.43
13:S:268:PHE:HD2	13:S:279:PRO:HG2	1.83	0.43
25:B:605:CLA:H61	25:B:605:CLA:H92	1.81	0.43
20:C:139:TRP:O	20:C:259:TYR:OH	2.36	0.43
25:C:610:CLA:H151	25:C:610:CLA:H112	1.54	0.43
33:m:101:LMG:H291	33:m:101:LMG:H322	1.56	0.43
9:f:25:VAL:HB	9:f:26:PRO:HD3	1.99	0.43
10:4:58:ARG:HA	10:4:61:MET:HE3	2.01	0.43
11:5:11:TRP:HZ3	24:5:305:CHL:HAA1	1.84	0.43
11:5:106:GLU:HG3	8:r:258:PHE:HD1	1.83	0.43
12:6:148:ILE:HA	12:6:151:ILE:HG22	2.00	0.43
12:6:200:LYS:HD3	25:6:315:CLA:HAA2	2.01	0.43
17:y:168:LYS:HD3	25:y:316:CLA:HBD	2.00	0.43
17:q:53:GLU:HB2	24:q:304:CHL:CHB	2.49	0.43
24:q:311:CHL:HBB1	24:q:311:CHL:HHC	2.00	0.43
25:b:602:CLA:HED3	25:b:603:CLA:H3A	2.00	0.43
19:a:273:PHE:CE1	30:d:408:LHG:HC61	2.54	0.43
25:a:604:CLA:H111	25:a:604:CLA:H151	1.90	0.43
20:c:439:ALA:HA	20:c:444:GLU:HB3	2.00	0.43
25:r:305:CLA:CHC	28:r:317:NEX:H362	2.49	0.43
12:7:101:THR:HA	12:7:104:LEU:HG	2.01	0.43
24:7:306:CHL:H143	24:7:306:CHL:H112	1.66	0.43
8:R:255:GLU:HG3	25:R:612:CLA:HED1	2.00	0.43
10:1:33:GLY:N	24:1:305:CHL:OBD	2.51	0.43
12:3:76:GLU:H	12:3:76:GLU:CD	2.26	0.43
13:S:199:GLU:CD	13:S:202:ARG:HH12	2.26	0.43
17:G:53:GLU:OE2	17:G:174:ARG:NE	2.37	0.43
17:G:124:MET:HE1	28:G:304:NEX:H32	2.00	0.43
24:G:313:CHL:H43	24:9:304:CHL:H2	2.00	0.43
17:8:52:LEU:O	17:8:56:HIS:ND1	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:8:312:CLA:H112	25:8:312:CLA:H72	1.71	0.43
25:C:601:CLA:H161	25:C:607:CLA:HMB3	2.00	0.43
17:g:27:GLU:OE1	17:g:27:GLU:N	2.50	0.43
25:q:305:CLA:HED1	24:q:311:CHL:H92	2.00	0.43
25:q:313:CLA:H143	25:q:313:CLA:H161	1.88	0.43
25:b:612:CLA:H141	25:b:612:CLA:H161	1.76	0.43
32:a:609:SQD:H292	32:a:609:SQD:H261	1.74	0.43
21:d:203:GLY:HA3	21:d:278:GLY:HA3	2.01	0.43
13:s:182:LEU:HD22	13:s:186:VAL:HG11	2.01	0.43
8:r:156:GLN:H	8:r:156:GLN:HG3	1.52	0.43
3:H:66:ILE:HD11	18:B:187:ALA:O	2.18	0.43
28:1:303:NEX:H11	28:1:303:NEX:H191	1.82	0.43
17:N:54:LEU:HD21	17:N:58:ARG:CZ	2.48	0.43
25:C:603:CLA:H193	25:C:603:CLA:H161	1.68	0.43
3:h:20:SER:N	3:h:21:PRO:HD2	2.33	0.43
4:i:28:PRO:O	4:i:31:ASN:ND2	2.49	0.43
33:m:101:LMG:H161	25:b:608:CLA:H2	2.00	0.43
10:4:168:LYS:HE3	25:4:314:CLA:HED2	2.00	0.43
11:5:59:TRP:CE2	24:5:312:CHL:HED2	2.54	0.43
11:5:123:ILE:CG2	28:5:304:NEX:C34	2.97	0.43
28:u:304:NEX:H30	24:u:312:CHL:HMA2	2.00	0.43
17:n:32:TYR:HB2	24:n:305:CHL:HMD3	2.01	0.43
17:n:151:ASP:OD1	29:n:301:0UR:O40	2.36	0.43
12:p:180:GLU:C	12:p:182:PHE:H	2.27	0.43
26:p:302:0IE:C13	24:p:306:CHL:HMC	2.49	0.43
18:b:464:PHE:HB2	21:d:280:TRP:CZ2	2.54	0.43
20:c:296:GLU:OE2	20:c:353:TRP:NE1	2.42	0.43
24:s:402:CHL:H3A	24:s:402:CHL:HBA1	1.52	0.43
12:7:44:LEU:HB2	12:7:48:SER:HB3	2.01	0.43
12:7:133:TYR:CE1	25:7:308:CLA:H2	2.54	0.43
8:R:88:GLN:HB3	19:A:230:ASN:HB3	2.01	0.43
8:R:109:VAL:HG22	8:R:111:THR:HG22	2.00	0.43
24:9:312:CHL:H2A	24:9:312:CHL:HED3	1.99	0.43
17:Y:110:ALA:HA	24:Y:308:CHL:CHC	2.49	0.43
17:8:168:LYS:HD3	25:8:313:CLA:HAA2	2.01	0.43
24:8:303:CHL:H3A	24:8:303:CHL:HBA1	1.45	0.43
18:B:462:PHE:HA	25:B:611:CLA:HMC1	2.00	0.43
19:A:140:ARG:HA	19:A:141:PRO:HD3	1.89	0.43
21:D:32:TRP:CD1	33:D:411:LMG:H152	2.54	0.43
21:D:153:PHE:CE1	35:D:403:PHO:H91	2.54	0.43
12:u:206:ARG:HA	12:u:209:MET:HE2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:n:312:CHL:H92	24:n:312:CHL:H62	1.73	0.43
17:y:147:GLY:C	17:y:149:ALA:H	2.26	0.43
12:p:44:LEU:HB2	12:p:48:SER:HB3	1.99	0.43
21:d:343:GLU:H	21:d:343:GLU:CD	2.27	0.43
8:r:44:ASP:OD1	8:r:44:ASP:N	2.52	0.43
12:7:45:GLY:O	12:7:48:SER:OG	2.37	0.43
8:R:86:LEU:HD13	18:B:13:LEU:HD23	2.00	0.42
25:R:612:CLA:H3A	25:R:612:CLA:HBA2	1.78	0.42
12:3:168:PRO:HG2	24:3:311:CHL:HBB2	2.01	0.42
17:N:104:ASN:HD22	17:N:107:LEU:HD13	1.84	0.42
17:Y:8:ARG:NE	17:Y:31:ASP:O	2.37	0.42
25:B:608:CLA:H93	25:B:608:CLA:H62	1.76	0.42
10:4:54:LEU:HD23	10:4:144:LEU:HB3	2.01	0.42
11:5:218:LYS:HE3	11:5:221:PHE:H	1.84	0.42
12:u:183:ASP:OD1	12:u:183:ASP:N	2.51	0.42
25:y:317:CLA:H61	25:y:317:CLA:H2	1.60	0.42
28:p:304:NEX:H382	25:p:308:CLA:HBA2	2.01	0.42
24:q:304:CHL:HBB1	24:q:304:CHL:CHC	2.46	0.42
18:b:174:ILE:HA	18:b:308:LYS:HD2	2.01	0.42
19:a:149:ALA:HB1	19:a:283:ILE:HB	2.01	0.42
19:a:269:ARG:HE	21:d:235:PHE:HB2	1.84	0.42
13:s:175:TRP:NE1	25:s:417:CLA:HBB1	2.34	0.42
24:r:307:CHL:HBB1	24:r:307:CHL:HHC	2.01	0.42
7:M:24:ILE:HG22	7:M:25:LEU:HD23	2.00	0.42
25:R:604:CLA:HMA2	24:R:605:CHL:C3C	2.50	0.42
18:B:338:VAL:HB	18:B:431:GLU:CD	2.44	0.42
19:A:10:GLY:HA3	19:A:15:GLU:CD	2.43	0.42
19:A:246:TYR:CE2	19:A:248:ILE:HG12	2.53	0.42
21:D:343:GLU:H	21:D:343:GLU:CD	2.28	0.42
22:W:109:ASP:O	22:W:111:ASN:N	2.52	0.42
17:g:131:ARG:HA	24:g:312:CHL:C4C	2.49	0.42
17:g:162:PHE:CZ	17:g:166:LYS:HD2	2.54	0.42
12:u:85:GLU:HB2	24:u:306:CHL:CHB	2.49	0.42
12:u:87:ILE:HG13	12:u:91:TRP:HD1	1.83	0.42
25:u:308:CLA:H43	24:u:310:CHL:HAA2	2.01	0.42
24:p:311:CHL:HHC	24:p:311:CHL:HBB1	2.01	0.42
17:q:115:ALA:O	17:q:119:THR:OG1	2.27	0.42
20:c:139:TRP:O	20:c:259:TYR:OH	2.36	0.42
20:c:334:THR:OG1	20:c:336:GLU:OE1	2.35	0.42
25:c:603:CLA:H62	25:c:603:CLA:H41	1.90	0.42
13:s:230:TYR:HB3	25:s:410:CLA:HED2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:195:SER:O	12:7:196:GLU:HB2	2.19	0.42
8:R:137:CYS:SG	8:R:240:MET:HA	2.60	0.42
10:1:74:GLU:HG2	10:1:84:ALA:HB1	2.02	0.42
12:3:142:ALA:HA	24:3:308:CHL:CHC	2.50	0.42
12:3:167:GLY:H	24:3:311:CHL:HMC	1.83	0.42
17:N:104:ASN:ND2	17:N:107:LEU:HD13	2.34	0.42
17:8:32:TYR:HB2	24:8:304:CHL:HMD3	2.02	0.42
24:8:304:CHL:H111	24:8:304:CHL:H91	1.82	0.42
25:C:601:CLA:H142	25:C:601:CLA:H112	1.79	0.42
30:D:408:LHG:H241	30:D:408:LHG:H272	1.81	0.42
25:g:315:CLA:H112	25:g:315:CLA:H72	1.85	0.42
17:y:21:PRO:HD2	17:y:24:LEU:HD12	2.01	0.42
17:y:125:GLY:CA	24:y:313:CHL:HAB	2.49	0.42
19:a:183:MET:HA	25:a:603:CLA:HMD1	2.00	0.42
25:a:603:CLA:H203	30:d:407:LHG:H162	2.01	0.42
35:a:606:PHO:HAB	21:d:205:LEU:HD13	2.00	0.42
20:c:210:GLY:HA3	20:c:214:SER:HB3	2.01	0.42
20:c:385:THR:HG1	20:c:386:HIS:CE1	2.37	0.42
13:s:68:LEU:HD21	13:s:249:GLU:HB3	2.00	0.42
25:s:411:CLA:C4D	25:s:412:CLA:HMD3	2.49	0.42
6:L:20:TRP:HZ2	30:D:407:LHG:HC91	1.84	0.42
10:1:58:ARG:HA	10:1:61:MET:HE3	2.01	0.42
25:S:616:CLA:H3A	25:S:616:CLA:HBA2	1.59	0.42
16:T:56:ILE:HD11	30:D:407:LHG:H301	2.01	0.42
17:G:59:TRP:CE2	24:G:312:CHL:HED2	2.54	0.42
17:N:23:TYR:OH	17:N:35:ASP:OD2	2.30	0.42
17:N:29:PRO:HG2	17:N:166:LYS:HE2	2.01	0.42
24:N:304:CHL:HBA1	24:N:304:CHL:H3A	1.67	0.42
18:B:464:PHE:HB2	21:D:280:TRP:CZ2	2.53	0.42
19:A:68:SER:HB3	21:D:313:THR:HG22	2.01	0.42
25:A:603:CLA:H142	25:A:603:CLA:H112	1.82	0.42
33:m:101:LMG:H161	33:m:101:LMG:H132	1.58	0.42
9:f:16:ARG:CZ	9:f:16:ARG:HA	2.50	0.42
12:6:53:PRO:HG2	12:6:67:ASP:HB3	2.01	0.42
12:6:218:GLN:O	12:6:222:THR:OG1	2.23	0.42
25:g:308:CLA:H42	24:g:310:CHL:HBD	2.01	0.42
25:q:306:CLA:C2B	28:s:401:NEX:C38	2.97	0.42
18:b:14:ASN:HB2	8:r:86:LEU:HD22	2.01	0.42
25:b:608:CLA:H93	25:b:608:CLA:H62	1.69	0.42
25:a:603:CLA:HBB1	25:a:603:CLA:HMB3	2.00	0.42
21:d:87:HIS:CE1	21:d:162:LEU:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:403:PHO:H2A	35:d:403:PHO:O2D	2.19	0.42
25:r:314:CLA:H3A	25:r:314:CLA:HBA2	1.43	0.42
12:7:80:GLN:H	12:7:80:GLN:HG2	1.67	0.42
12:7:122:GLY:C	12:7:124:GLN:H	2.28	0.42
24:7:310:CHL:HMB2	24:7:313:CHL:HMC	2.01	0.42
6:L:5:ASN:ND2	18:B:15:ASP:OD2	2.43	0.42
8:R:169:TYR:HB2	8:R:174:LEU:HD21	2.01	0.42
8:R:260:SER:HA	25:R:612:CLA:HED2	2.01	0.42
28:1:303:NEX:H222	25:1:307:CLA:C4B	2.50	0.42
11:2:10:LEU:O	24:2:305:CHL:HBC2	2.19	0.42
25:2:308:CLA:H2A	25:2:308:CLA:O1D	2.19	0.42
13:S:182:LEU:HD22	13:S:186:VAL:HG11	2.01	0.42
17:Y:136:PRO:HB2	24:Y:311:CHL:HBB2	2.01	0.42
17:8:135:GLY:H	24:8:309:CHL:HMC	1.83	0.42
18:B:395:VAL:HG23	18:B:397:VAL:HG13	2.02	0.42
25:B:604:CLA:H42	25:B:605:CLA:H2	2.01	0.42
33:i:101:LMG:H111	25:a:607:CLA:HAA2	2.01	0.42
25:g:314:CLA:H43	25:g:316:CLA:HBA1	2.00	0.42
28:y:304:NEX:H241	25:y:308:CLA:O2A	2.18	0.42
18:b:463:PHE:CE1	18:b:467:ILE:HD11	2.54	0.42
8:R:78:PHE:N	8:R:102:PHE:O	2.44	0.42
10:1:101:TYR:O	10:1:107:LEU:HD12	2.20	0.42
12:3:90:ARG:HA	12:3:93:MET:HE3	2.01	0.42
24:G:313:CHL:HHC	24:9:304:CHL:H52	2.01	0.42
24:9:305:CHL:H62	24:9:305:CHL:H101	1.82	0.42
24:9:310:CHL:HHC	24:9:310:CHL:HBB1	2.02	0.42
17:Y:162:PHE:CE2	17:Y:166:LYS:HD2	2.55	0.42
17:8:110:ALA:HA	24:8:307:CHL:CHC	2.49	0.42
18:B:174:ILE:HA	18:B:308:LYS:HD2	2.02	0.42
25:B:608:CLA:ND	33:B:619:LMG:H121	2.34	0.42
35:A:606:PHO:HAB	21:D:205:LEU:HD13	2.00	0.42
5:k:28:LEU:HB3	31:v:401:8CT:C18	2.49	0.42
11:5:10:LEU:O	24:5:305:CHL:HBC2	2.20	0.42
12:6:217:VAL:O	12:6:221:VAL:HG22	2.20	0.42
24:n:304:CHL:H41	24:n:304:CHL:H61	1.74	0.42
12:p:248:ILE:HB	12:p:252:ALA:H	1.84	0.42
22:w:96:TRP:CH2	33:w:201:LMG:HC91	2.55	0.42
25:b:612:CLA:H93	25:b:612:CLA:H111	1.78	0.42
21:d:263:ASN:HB3	21:d:266:TRP:HB3	2.01	0.42
13:s:95:SER:OG	13:s:97:GLU:OE1	2.31	0.42
8:r:169:TYR:HB2	8:r:174:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:116:PRO:O	12:7:117:VAL:C	2.62	0.42
28:7:304:NEX:H392	25:7:308:CLA:CMB	2.49	0.42
24:7:311:CHL:HHC	24:7:311:CHL:HBB1	2.01	0.42
7:M:9:ILE:HD11	7:m:8:LEU:C	2.45	0.42
12:9:183:ASP:OD1	12:9:183:ASP:N	2.52	0.42
17:N:178:PHE:HE2	25:N:316:CLA:HAB	1.83	0.42
17:Y:145:TYR:HB3	25:Y:313:CLA:HED2	2.01	0.42
10:4:209:ASN:HB3	24:4:317:CHL:HED2	2.00	0.42
28:5:304:NEX:H201	28:5:304:NEX:H15	1.62	0.42
12:6:171:GLU:HB3	12:6:172:PRO:HD2	2.02	0.42
17:n:134:GLY:HA2	24:n:311:CHL:HAC1	2.01	0.42
24:y:305:CHL:H51	24:y:305:CHL:H12	1.69	0.42
17:q:69:THR:OG1	17:q:70:PRO:HD3	2.20	0.42
17:q:106:SER:OG	13:s:148:ALA:N	2.53	0.42
17:q:110:ALA:HA	24:q:307:CHL:CHC	2.49	0.42
19:a:166:GLY:HA3	20:c:346:PHE:HE1	1.84	0.42
32:a:609:SQD:H441	32:a:609:SQD:H2	1.70	0.42
25:c:601:CLA:H161	25:c:607:CLA:HMB3	2.01	0.42
21:d:153:PHE:CE1	35:d:403:PHO:H91	2.55	0.42
12:7:200:LYS:HD3	25:7:316:CLA:HBD	2.01	0.42
5:K:22:LEU:O	5:K:25:ILE:HG12	2.20	0.42
8:R:242:ALA:C	25:R:612:CLA:HBC1	2.45	0.42
24:2:305:CHL:O1D	30:2:319:LHG:H102	2.20	0.42
24:S:605:CHL:HBC2	24:S:606:CHL:HHD	2.02	0.42
24:G:310:CHL:HBC2	24:G:311:CHL:HHD	2.01	0.42
12:9:78:PHE:O	12:9:82:ARG:NH1	2.52	0.42
12:9:190:ASP:HB2	12:9:193:THR:HB	2.02	0.42
17:Y:133:SER:OG	12:7:50:GLY:N	2.43	0.42
17:8:59:TRP:CE2	24:8:309:CHL:HED2	2.55	0.42
18:B:92:SER:OG	18:B:93:TYR:N	2.52	0.42
25:B:615:CLA:H141	25:B:615:CLA:H161	1.87	0.42
25:D:405:CLA:H161	25:D:405:CLA:H143	1.77	0.42
10:4:104:ASN:HB3	10:4:107:LEU:HG	2.02	0.42
25:5:308:CLA:H2A	25:5:308:CLA:O1D	2.19	0.42
16:t:52:LEU:HD11	30:d:407:LHG:H171	2.02	0.42
25:u:317:CLA:H11	25:u:317:CLA:C4D	2.50	0.42
12:p:122:GLY:C	12:p:124:GLN:H	2.28	0.42
24:p:305:CHL:HBA1	24:p:305:CHL:H3A	1.72	0.42
25:p:317:CLA:H11	25:p:317:CLA:C4D	2.49	0.42
17:q:125:GLY:HA2	24:q:311:CHL:HAB	2.02	0.42
18:b:156:PHE:HB3	18:b:162:PHE:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:604:CLA:H93	25:b:604:CLA:H61	1.77	0.42
25:b:610:CLA:H151	25:b:615:CLA:HBD	2.01	0.42
19:a:14:TRP:NE1	19:a:18:CYS:SG	2.93	0.42
25:c:608:CLA:O1D	30:d:408:LHG:HC12	2.20	0.42
13:s:128:ARG:HA	13:s:131:MET:HE3	2.00	0.42
10:1:51:GLU:HG2	24:1:312:CHL:HED2	2.02	0.42
10:1:194:PRO:HA	10:1:197:CYS:HB2	2.02	0.42
12:3:171:GLU:HB3	12:3:172:PRO:HD2	2.02	0.42
13:S:230:TYR:HB3	25:S:609:CLA:HED2	2.01	0.42
12:9:102:PRO:O	12:9:116:PRO:HB2	2.20	0.42
17:N:59:TRP:CD1	24:N:312:CHL:HMD3	2.55	0.42
24:Y:305:CHL:H142	24:Y:305:CHL:H112	1.72	0.42
24:Y:317:CHL:HAB	20:C:194:PRO:HG3	2.02	0.42
18:B:247:TRP:HB2	25:B:612:CLA:HBC1	2.02	0.42
25:B:613:CLA:H143	25:B:613:CLA:H111	1.75	0.42
19:A:55:ALA:O	19:A:70:SER:OG	2.28	0.42
19:A:93:PHE:HZ	25:A:607:CLA:HAA1	1.84	0.42
20:C:136:GLY:O	20:C:144:LYS:NZ	2.49	0.42
20:C:288:GLU:OE1	20:C:288:GLU:N	2.44	0.42
28:4:303:NEX:H201	28:4:303:NEX:H15	1.62	0.42
11:5:121:VAL:HG23	24:5:313:CHL:HBB2	2.01	0.42
12:6:233:HIS:CG	25:6:316:CLA:HAA2	2.55	0.42
24:y:318:CHL:HAB	20:c:194:PRO:HG3	2.01	0.42
33:w:201:LMG:H152	33:w:201:LMG:H182	1.33	0.42
18:b:247:TRP:HB2	25:b:612:CLA:HBC1	2.02	0.42
24:s:403:CHL:HHC	24:s:403:CHL:HBB1	2.02	0.42
28:r:317:NEX:H201	28:r:317:NEX:H15	1.62	0.42
1:Z:30:PRO:HD3	15:V:304:ASP:OD2	2.20	0.42
2:E:66:PHE:CZ	2:E:75:VAL:HG11	2.54	0.42
27:R:615:XAT:H35	27:R:615:XAT:H401	1.80	0.42
10:1:155:MET:HB2	25:1:313:CLA:O1A	2.20	0.42
10:1:168:LYS:HE3	25:1:314:CLA:HED2	2.02	0.42
24:8:303:CHL:H61	24:8:303:CHL:H41	1.63	0.42
18:B:18:ARG:HD2	18:B:115:TRP:CE3	2.55	0.42
25:B:610:CLA:H151	25:B:615:CLA:HBD	2.02	0.42
19:A:140:ARG:NH1	21:D:219:GLU:O	2.50	0.42
10:4:188:LEU:HD13	10:4:188:LEU:HA	1.91	0.42
11:5:136:PRO:HB2	24:5:312:CHL:HBB2	2.02	0.42
17:g:59:TRP:CE2	24:g:312:CHL:HED2	2.54	0.42
12:p:102:PRO:O	12:p:113:LEU:HD13	2.20	0.42
12:p:116:PRO:O	12:p:117:VAL:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:304:NEX:C33	24:p:310:CHL:O2A	2.68	0.42
25:p:307:CLA:HMD2	24:q:303:CHL:H2	2.02	0.42
17:q:164:GLU:HG2	17:q:168:LYS:HE3	2.02	0.42
25:b:604:CLA:H12	25:b:605:CLA:C1D	2.49	0.42
8:r:47:TRP:HE3	24:r:302:CHL:HAA1	1.83	0.42
12:7:79:LYS:HA	12:7:82:ARG:CZ	2.50	0.42
27:R:615:XAT:H173	27:R:615:XAT:H3	1.85	0.41
13:S:148:ALA:N	17:8:106:SER:OG	2.53	0.41
13:S:175:TRP:NE1	25:S:616:CLA:HBB1	2.35	0.41
13:S:212:ALA:O	13:S:214:GLY:N	2.44	0.41
24:G:310:CHL:HMB1	24:G:313:CHL:HMC	2.02	0.41
24:N:312:CHL:H92	24:N:312:CHL:H62	1.73	0.41
17:Y:101:TYR:O	17:Y:107:LEU:HD12	2.20	0.41
18:B:87:ASN:OD1	18:B:87:ASN:N	2.53	0.41
20:C:26:GLY:HA3	25:C:611:CLA:HMD2	2.01	0.41
22:W:104:LYS:HD3	22:W:104:LYS:HA	1.76	0.41
28:4:303:NEX:H28	24:4:309:CHL:CBA	2.50	0.41
11:5:29:PRO:HG2	11:5:166:LYS:HE2	2.01	0.41
28:5:304:NEX:H35	28:5:304:NEX:H401	1.57	0.41
17:n:98:GLY:HA3	17:n:110:ALA:O	2.20	0.41
18:b:18:ARG:HD2	18:b:115:TRP:CE3	2.55	0.41
19:a:104:GLU:O	19:a:105:TRP:C	2.61	0.41
28:7:304:NEX:H201	28:7:304:NEX:H15	1.62	0.41
3:H:55:GLU:HB3	3:H:60:ASP:HB2	2.02	0.41
4:I:9:TYR:HD2	22:W:88:LEU:HD11	1.83	0.41
17:G:194:PRO:O	29:G:301:0UR:O39	2.38	0.41
17:N:155:MET:HB3	25:N:313:CLA:O1A	2.20	0.41
25:Y:306:CLA:H12	12:7:71:LEU:HD11	2.02	0.41
19:A:329:GLU:HG3	20:C:399:ALA:HB2	2.01	0.41
20:C:29:ARG:NH1	25:C:611:CLA:OBD	2.49	0.41
20:C:389:LEU:HD13	20:C:397:GLY:N	2.34	0.41
7:m:24:ILE:HG22	7:m:25:LEU:HD23	2.01	0.41
16:t:56:ILE:HD11	30:d:407:LHG:H331	2.01	0.41
25:g:307:CLA:H12	12:u:71:LEU:HD11	2.01	0.41
12:u:77:MET:HA	12:u:80:GLN:OE1	2.20	0.41
12:u:91:TRP:O	12:u:95:GLY:N	2.54	0.41
12:u:190:ASP:HB2	12:u:193:THR:HB	2.02	0.41
25:u:314:CLA:H43	25:u:316:CLA:HBA1	2.02	0.41
17:n:29:PRO:HG2	17:n:166:LYS:HE2	2.01	0.41
12:p:91:TRP:CE2	24:p:312:CHL:HED2	2.55	0.41
18:b:395:VAL:HG23	18:b:397:VAL:HG13	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:269:ARG:HH11	21:d:222:LEU:HD13	1.85	0.41
25:c:609:CLA:H112	25:c:609:CLA:H142	1.63	0.41
1:Z:1:MET:SD	1:Z:1:MET:N	2.81	0.41
1:Z:32:GLY:HA2	1:Z:35:GLU:HG2	2.02	0.41
9:F:12:ILE:HB	9:F:15:VAL:HG12	2.01	0.41
12:3:218:GLN:HG2	12:3:229:ASN:ND2	2.35	0.41
24:G:305:CHL:H3A	24:G:305:CHL:HBA1	1.36	0.41
12:9:209:MET:HB2	24:9:305:CHL:OMC	2.21	0.41
25:9:313:CLA:H43	25:9:315:CLA:HBA1	2.02	0.41
17:Y:11:TRP:CG	17:Y:34:TRP:HB2	2.56	0.41
17:Y:125:GLY:CA	24:Y:312:CHL:HAB	2.49	0.41
17:8:45:THR:HG22	17:8:49:ASN:ND2	2.34	0.41
18:B:198:ILE:HG23	18:B:202:HIS:CE1	2.54	0.41
25:B:604:CLA:H12	25:B:605:CLA:C1D	2.50	0.41
19:A:84:PRO:HA	19:A:112:TYR:CG	2.56	0.41
19:A:276:ALA:HB2	21:D:215:GLY:C	2.45	0.41
32:D:409:SQD:H291	33:D:411:LMG:C22	2.50	0.41
3:h:58:ASN:O	3:h:59:SER:OG	2.37	0.41
10:4:73:LEU:O	10:4:78:GLY:N	2.53	0.41
10:4:151:ASP:OD1	29:4:301:0UR:O40	2.38	0.41
12:u:209:MET:HE3	24:u:306:CHL:OMC	2.20	0.41
17:n:162:PHE:CZ	17:n:166:LYS:HD2	2.56	0.41
26:p:302:0IE:C14	24:p:306:CHL:HMC	2.50	0.41
24:p:305:CHL:H51	24:p:305:CHL:H12	1.68	0.41
17:q:58:ARG:NH1	24:q:310:CHL:OBD	2.46	0.41
18:b:435:ALA:C	18:b:437:LEU:H	2.27	0.41
25:b:612:CLA:H41	25:b:612:CLA:H61	1.43	0.41
25:b:615:CLA:H152	25:b:615:CLA:H112	1.85	0.41
20:c:285:TYR:O	20:c:411:ARG:NH2	2.51	0.41
20:c:327:LYS:C	20:c:329:LEU:H	2.28	0.41
13:s:58:TRP:O	13:s:60:GLY:N	2.52	0.41
13:s:124:LEU:O	13:s:128:ARG:HG3	2.20	0.41
13:s:199:GLU:OE2	13:s:202:ARG:NH2	2.37	0.41
8:r:137:CYS:SG	8:r:240:MET:HA	2.60	0.41
2:E:71:LEU:O	2:E:75:VAL:HG12	2.21	0.41
24:1:304:CHL:OBD	24:1:305:CHL:HHD	2.20	0.41
12:3:103:GLU:OE2	12:3:228:GLU:HG2	2.20	0.41
24:3:309:CHL:CBA	28:3:318:NEX:H31	2.50	0.41
25:9:314:CLA:H72	25:9:315:CLA:ND	2.34	0.41
17:N:40:SER:HA	17:N:45:THR:HG23	2.02	0.41
18:B:74:SER:HG	18:B:78:TRP:CG	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:608:CLA:C4A	25:B:608:CLA:HBA2	2.51	0.41
19:A:149:ALA:HB1	19:A:283:ILE:HB	2.01	0.41
20:C:86:GLY:O	20:C:94:VAL:N	2.50	0.41
20:C:327:LYS:C	20:C:329:LEU:H	2.29	0.41
35:D:403:PHO:H2A	35:D:403:PHO:O2D	2.21	0.41
10:4:69:THR:OG1	10:4:70:PRO:HD3	2.20	0.41
10:4:155:MET:HB2	25:4:313:CLA:O1A	2.20	0.41
11:5:47:ARG:NH2	11:5:48:ARG:HE	2.18	0.41
12:6:108:TYR:HD1	12:6:108:TYR:HA	1.80	0.41
12:6:152:GLN:HE22	24:6:310:CHL:HAC1	1.85	0.41
17:y:136:PRO:HB2	24:y:312:CHL:HBB2	2.02	0.41
25:y:315:CLA:HBD	25:y:316:CLA:OBD	2.20	0.41
18:b:9:HIS:HB3	25:b:606:CLA:HAB	2.01	0.41
18:b:278:GLY:O	18:b:280:PHE:N	2.53	0.41
18:b:437:LEU:HD23	18:b:437:LEU:HA	1.92	0.41
25:b:606:CLA:H72	25:b:606:CLA:H12	2.02	0.41
20:c:203:LYS:HG2	20:c:209:ASP:HB3	2.02	0.41
25:c:607:CLA:H141	25:c:607:CLA:H162	1.87	0.41
25:c:612:CLA:HBA1	25:c:612:CLA:HBD	2.02	0.41
10:1:99:LEU:HB3	10:1:110:ALA:HB3	2.02	0.41
11:2:29:PRO:HG2	11:2:166:LYS:HE2	2.01	0.41
11:2:107:LEU:HD23	11:2:107:LEU:HA	1.88	0.41
28:2:304:NEX:H21	17:N:153:MET:HA	2.03	0.41
12:3:76:GLU:HA	12:3:79:LYS:HE3	2.02	0.41
12:3:143:GLN:N	24:3:308:CHL:OMC	2.48	0.41
24:G:313:CHL:H62	24:G:313:CHL:H92	1.76	0.41
12:9:141:HIS:CG	12:9:143:GLN:HE22	2.38	0.41
12:9:212:MET:HE2	26:9:302:0IE:C4	2.50	0.41
20:C:343:THR:O	20:C:343:THR:OG1	2.39	0.41
21:D:160:TYR:HA	21:D:290:ALA:HB2	2.02	0.41
21:D:271:MET:HE2	21:D:271:MET:HB3	1.92	0.41
11:5:30:GLY:O	11:5:174:ARG:NH2	2.48	0.41
28:5:304:NEX:H11	28:5:304:NEX:H191	1.82	0.41
12:6:171:GLU:O	12:6:173:THR:N	2.50	0.41
28:g:304:NEX:H35	28:g:304:NEX:H401	1.58	0.41
12:u:141:HIS:CG	12:u:143:GLN:HE22	2.38	0.41
12:p:34:GLU:O	12:p:40:ARG:HA	2.19	0.41
25:p:315:CLA:H2A	25:p:315:CLA:O2D	2.19	0.41
25:b:613:CLA:H62	25:b:613:CLA:H41	1.54	0.41
19:a:84:PRO:HA	19:a:112:TYR:CG	2.56	0.41
19:a:161:TYR:HB3	19:a:162:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:276:ALA:HB2	21:d:215:GLY:C	2.45	0.41
20:c:26:GLY:HA3	25:c:611:CLA:HMD2	2.02	0.41
20:c:142:LYS:HD3	20:c:249:ARG:HG2	2.03	0.41
2:E:97:ASP:O	2:E:101:ALA:HB2	2.21	0.41
3:H:26:TYR:HE2	8:R:83:ILE:HG12	1.85	0.41
8:R:63:GLY:O	8:R:237:ARG:NH1	2.51	0.41
8:R:104:THR:HG23	8:R:119:GLU:HG3	2.02	0.41
8:R:243:PHE:CD2	27:R:615:XAT:H12	2.56	0.41
10:1:209:ASN:HB3	24:1:317:CHL:HED2	2.02	0.41
12:3:217:VAL:O	12:3:218:GLN:C	2.64	0.41
13:S:123:GLU:HB2	24:S:602:CHL:CHB	2.50	0.41
12:9:85:GLU:HB2	24:9:305:CHL:CHB	2.50	0.41
17:N:83:GLU:OE1	17:N:88:LYS:HB3	2.21	0.41
17:8:184:PHE:O	17:8:187:SER:OG	2.30	0.41
24:8:304:CHL:HBB1	24:8:304:CHL:CHC	2.46	0.41
25:B:604:CLA:HBB1	25:B:613:CLA:HBC3	2.03	0.41
21:D:178:ILE:O	21:D:182:ILE:HG13	2.21	0.41
22:W:75:ARG:H	22:W:75:ARG:HD2	1.84	0.41
3:h:55:GLU:HB3	3:h:60:ASP:HB2	2.03	0.41
10:4:108:VAL:HG13	24:4:308:CHL:C1D	2.50	0.41
24:5:305:CHL:O1D	30:5:319:LHG:H102	2.20	0.41
12:u:131:ILE:O	12:u:141:HIS:HA	2.20	0.41
17:n:53:GLU:HB2	24:n:305:CHL:CHB	2.50	0.41
25:b:603:CLA:H112	25:b:603:CLA:H91	1.81	0.41
19:a:37:ARG:HH12	30:d:407:LHG:H383	1.84	0.41
20:c:343:THR:O	20:c:343:THR:OG1	2.39	0.41
21:d:180:ARG:NH1	21:d:333:ASP:OD1	2.54	0.41
1:Z:2:ILE:O	1:Z:6:GLN:HG2	2.20	0.41
2:E:79:PRO:HD3	21:D:56:THR:HG21	2.02	0.41
11:2:11:TRP:HZ3	24:2:305:CHL:HAA1	1.86	0.41
17:G:9:ALA:HB1	24:G:305:CHL:HBC1	2.03	0.41
12:9:85:GLU:N	24:9:305:CHL:HMB2	2.35	0.41
28:N:303:NEX:H23	25:N:307:CLA:H43	2.01	0.41
17:Y:4:TYR:OH	17:Y:163:ALA:O	2.39	0.41
17:8:125:GLY:HA2	24:8:310:CHL:HAB	2.01	0.41
25:B:611:CLA:H71	30:A:601:LHG:H312	2.02	0.41
25:B:611:CLA:H192	25:B:611:CLA:H162	1.82	0.41
19:A:161:TYR:HB3	19:A:162:PRO:HD3	2.02	0.41
20:C:395:VAL:HG23	20:C:407:PHE:N	2.35	0.41
10:4:101:TYR:O	10:4:107:LEU:HD12	2.21	0.41
28:4:303:NEX:C22	25:4:307:CLA:CHC	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:y:302:0IE:C13	24:y:306:CHL:HBB1	2.51	0.41
19:a:68:SER:OG	19:a:69:GLY:N	2.50	0.41
19:a:121:LEU:HD13	19:a:121:LEU:HA	1.85	0.41
19:a:184:ILE:HG23	19:a:328:MET:SD	2.61	0.41
21:d:146:PHE:C	21:d:149:PRO:HD2	2.46	0.41
25:d:405:CLA:H161	25:d:405:CLA:H202	1.67	0.41
13:s:76:ARG:HD3	13:s:96:GLY:HA3	2.03	0.41
13:s:253:LYS:HD3	25:s:412:CLA:HAA2	2.03	0.41
24:s:406:CHL:HBC2	24:s:407:CHL:HHD	2.02	0.41
8:r:69:PRO:C	8:r:71:CYS:N	2.79	0.41
25:7:317:CLA:H11	25:7:317:CLA:C4D	2.51	0.41
10:1:8:ARG:CZ	10:1:26:GLY:H	2.33	0.41
13:S:271:GLN:HG2	13:S:271:GLN:H	1.58	0.41
17:G:168:LYS:HD3	25:G:316:CLA:HBD	2.03	0.41
12:9:94:LEU:HG	25:9:307:CLA:HAB	2.02	0.41
18:B:9:HIS:HB3	25:B:606:CLA:HAB	2.02	0.41
18:B:315:ILE:HG13	18:B:321:LYS:HG3	2.02	0.41
18:B:380:ASP:N	18:B:380:ASP:OD1	2.54	0.41
25:B:612:CLA:H111	25:B:612:CLA:H93	1.77	0.41
19:A:37:ARG:HH11	19:A:41:LEU:HD12	1.84	0.41
19:A:140:ARG:HD2	20:C:444:GLU:O	2.19	0.41
37:C:620:DGD:HB22	37:C:620:DGD:HB52	1.46	0.41
10:4:28:PHE:O	10:4:31:ASP:HB2	2.21	0.41
12:6:169:LEU:HB2	24:6:311:CHL:HBB1	2.02	0.41
25:6:307:CLA:H2A	25:6:307:CLA:O1D	2.21	0.41
17:g:58:ARG:NE	17:g:169:GLU:OE2	2.42	0.41
17:g:123:LEU:HD13	17:g:123:LEU:HA	1.88	0.41
12:p:144:SER:N	24:p:309:CHL:OMC	2.54	0.41
12:p:163:ARG:HG3	24:p:312:CHL:C1D	2.51	0.41
28:p:304:NEX:C24	25:p:308:CLA:O2A	2.67	0.41
25:a:603:CLA:H122	25:a:603:CLA:H162	1.86	0.41
30:a:612:LHG:HC12	21:d:269:PHE:CG	2.55	0.41
20:c:86:GLY:O	20:c:94:VAL:N	2.50	0.41
25:c:601:CLA:H143	25:c:601:CLA:H162	1.82	0.41
28:r:301:NEX:H35	28:r:301:NEX:H401	1.75	0.41
2:E:45:SER:HB2	2:E:48:TYR:HB3	2.03	0.41
2:E:95:ILE:O	21:D:84:SER:OG	2.24	0.41
6:L:34:SER:HB3	19:A:78:ILE:HD13	2.03	0.41
8:R:112:GLU:C	8:R:114:LEU:H	2.29	0.41
8:R:131:LEU:O	8:R:135:ARG:HG3	2.21	0.41
9:F:25:VAL:HB	9:F:26:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1:68:LEU:O	10:1:72:ALA:N	2.53	0.41
10:1:130:TYR:OH	28:1:303:NEX:H192	2.20	0.41
12:3:53:PRO:HG2	12:3:67:ASP:HB3	2.02	0.41
13:S:58:TRP:CD1	17:8:130:TYR:HH	2.39	0.41
13:S:104:TYR:HB3	24:S:602:CHL:C3D	2.51	0.41
13:S:199:GLU:OE2	13:S:202:ARG:NH2	2.37	0.41
24:G:313:CHL:H111	24:G:313:CHL:H143	1.86	0.41
12:9:87:ILE:HG13	12:9:91:TRP:HD1	1.85	0.41
12:9:100:LEU:HD12	12:9:101:THR:HG22	2.03	0.41
25:9:314:CLA:O2D	25:9:314:CLA:H2A	2.20	0.41
17:N:32:TYR:HB2	24:N:305:CHL:HMD3	2.02	0.41
17:Y:54:LEU:HD23	17:Y:144:LEU:HD22	2.03	0.41
17:Y:58:ARG:NE	17:Y:169:GLU:OE2	2.41	0.41
17:Y:83:GLU:HB2	17:Y:92:GLN:HG3	2.03	0.41
26:Y:302:0IE:C13	24:Y:305:CHL:HBB1	2.51	0.41
24:Y:312:CHL:HAA2	12:7:68:THR:HG21	2.03	0.41
25:Y:313:CLA:HBB1	25:Y:313:CLA:HMB3	2.02	0.41
25:8:305:CLA:H41	25:7:307:CLA:H51	2.03	0.41
18:B:460:LEU:O	18:B:463:PHE:HB3	2.21	0.41
19:A:93:PHE:CD2	19:A:95:PRO:HD3	2.56	0.41
19:A:135:PHE:CE1	20:C:437:ARG:HG3	2.56	0.41
19:A:149:ALA:HB3	19:A:150:PRO:HD3	2.02	0.41
19:A:316:THR:OG1	19:A:317:TRP:N	2.54	0.41
20:C:210:GLY:O	20:C:211:TRP:C	2.64	0.41
6:l:13:LEU:HD22	7:m:25:LEU:HB2	2.02	0.41
10:4:21:PRO:HG3	10:4:35:ASP:HB3	2.03	0.41
10:4:57:ALA:HB2	10:4:177:MET:HE2	2.02	0.41
10:4:70:PRO:HG3	25:4:307:CLA:C1D	2.51	0.41
11:5:11:TRP:HB3	11:5:32:TYR:HB3	2.02	0.41
24:5:312:CHL:C4A	24:5:312:CHL:HBA2	2.50	0.41
25:5:314:CLA:H43	25:5:316:CLA:HBA1	2.03	0.41
12:6:90:ARG:HA	12:6:93:MET:HE3	2.02	0.41
12:6:213:PHE:HD1	25:6:306:CLA:HBB2	1.85	0.41
17:g:10:LEU:HD13	17:g:16:SER:HB2	2.03	0.41
24:g:305:CHL:H162	24:g:305:CHL:H122	1.77	0.41
24:g:305:CHL:HAC1	30:g:319:LHG:HC31	2.03	0.41
24:g:306:CHL:H62	24:g:306:CHL:H92	1.72	0.41
12:u:93:MET:O	12:u:96:THR:OG1	2.39	0.41
17:n:51:GLU:O	17:n:55:ILE:HG12	2.21	0.41
17:y:11:TRP:CG	17:y:34:TRP:HB2	2.55	0.41
17:y:39:LEU:HD11	25:q:305:CLA:H12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:192:LYS:NZ	17:y:200:GLU:OE2	2.35	0.41
28:y:304:NEX:H15	28:y:304:NEX:H201	1.62	0.41
12:p:164:CYS:HB3	17:q:19:ALA:HB2	2.02	0.41
17:q:23:TYR:OH	17:q:35:ASP:OD2	2.35	0.41
22:w:93:SER:HA	22:w:96:TRP:HB3	2.03	0.41
18:b:71:ILE:HD11	25:b:607:CLA:C2A	2.51	0.41
32:a:609:SQD:H1	21:d:232:PHE:HB3	2.01	0.41
21:d:271:MET:HE2	21:d:271:MET:HB3	1.91	0.41
30:d:408:LHG:H271	30:d:408:LHG:H302	1.72	0.41
13:s:199:GLU:CD	13:s:202:ARG:HH12	2.28	0.41
8:r:56:TRP:NE1	8:r:68:ASP:OD2	2.46	0.41
28:7:304:NEX:H401	28:7:304:NEX:H35	1.58	0.41
10:1:126:LEU:HB2	28:1:303:NEX:H203	2.03	0.41
17:G:27:GLU:OE1	17:G:27:GLU:N	2.48	0.41
17:G:52:LEU:O	17:G:56:HIS:ND1	2.55	0.41
17:G:110:ALA:HA	24:G:309:CHL:CHC	2.51	0.41
17:G:120:GLN:HE22	24:G:311:CHL:CMC	2.34	0.41
25:G:307:CLA:H12	12:9:71:LEU:HD11	2.03	0.41
28:9:319:NEX:H201	28:9:319:NEX:H15	1.62	0.41
17:N:68:LEU:HD22	17:N:68:LEU:HA	1.94	0.41
25:B:608:CLA:C1D	33:B:619:LMG:H121	2.51	0.41
19:A:184:ILE:HG23	19:A:328:MET:SD	2.61	0.41
21:D:229:ALA:O	30:D:408:LHG:O1	2.34	0.41
2:e:103:GLU:HA	2:e:106:LYS:HD2	2.03	0.41
30:4:318:LHG:H142	30:4:318:LHG:H172	1.91	0.41
12:6:107:LYS:HB3	12:6:107:LYS:HE2	1.88	0.41
28:6:303:NEX:C28	24:6:309:CHL:H3A	2.51	0.41
16:t:37:GLU:C	16:t:39:LEU:H	2.29	0.41
17:g:147:GLY:C	17:g:149:ALA:H	2.29	0.41
12:u:98:GLY:H	12:u:101:THR:HG23	1.86	0.41
25:b:610:CLA:H102	25:b:615:CLA:HAA1	2.03	0.41
19:a:267:ASN:ND2	21:d:232:PHE:O	2.54	0.41
20:c:213:VAL:HG23	37:c:619:DGD:HD61	2.03	0.41
25:c:607:CLA:H142	25:c:607:CLA:H111	1.81	0.41
35:d:403:PHO:H72	25:d:404:CLA:H111	2.03	0.41
13:s:119:LEU:HD13	13:s:119:LEU:HA	1.87	0.41
25:s:411:CLA:HBD	25:s:412:CLA:OBD	2.21	0.41
8:r:93:ASN:OD1	8:r:93:ASN:N	2.54	0.41
8:r:261:LEU:HD12	8:r:261:LEU:HA	1.82	0.41
12:7:125:ILE:HG12	12:7:145:ILE:HB	2.02	0.41
1:Z:20:VAL:HG13	25:C:611:CLA:H143	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:GLN:OE1	19:A:312:ARG:NH1	2.54	0.40
10:1:10:LEU:HG	10:1:20:VAL:HG11	2.03	0.40
10:1:201:HIS:HA	10:1:208:ASN:HB3	2.02	0.40
12:3:209:MET:HB2	24:3:305:CHL:HMC	2.03	0.40
24:S:602:CHL:HHC	24:S:602:CHL:HBB1	2.02	0.40
17:N:137:LEU:HG	24:N:311:CHL:HBB1	2.03	0.40
17:Y:188:LEU:HD12	17:Y:218:PHE:HD2	1.86	0.40
18:B:463:PHE:CE1	18:B:467:ILE:HD11	2.55	0.40
25:D:405:CLA:H112	25:D:405:CLA:H142	1.79	0.40
30:4:318:LHG:H111	30:4:318:LHG:HC82	1.80	0.40
12:6:66:TRP:CZ3	24:6:304:CHL:HBD	2.56	0.40
24:6:311:CHL:HBB1	24:6:311:CHL:CHC	2.51	0.40
12:u:78:PHE:CZ	12:u:82:ARG:HD3	2.56	0.40
12:u:168:PRO:HG3	28:u:304:NEX:H192	2.02	0.40
17:y:81:PHE:CE1	17:y:102:LEU:HA	2.57	0.40
19:a:93:PHE:HZ	25:a:607:CLA:HAA1	1.86	0.40
20:c:433:ALA:HA	25:c:605:CLA:HED2	2.03	0.40
21:d:146:PHE:O	21:d:149:PRO:HD2	2.21	0.40
12:7:189:ALA:O	12:7:194:PHE:HB2	2.20	0.40
28:7:304:NEX:C32	24:7:310:CHL:H3A	2.51	0.40
8:R:130:GLU:HB2	24:R:602:CHL:C1B	2.51	0.40
24:2:312:CHL:C4A	24:2:312:CHL:HBA2	2.50	0.40
24:3:309:CHL:H3A	28:3:318:NEX:C28	2.51	0.40
28:S:617:NEX:H222	25:8:306:CLA:CHC	2.52	0.40
12:9:76:GLU:CD	17:N:41:ALA:HB1	2.47	0.40
24:9:311:CHL:HMA1	28:9:319:NEX:C32	2.51	0.40
17:N:12:LEU:HD12	24:N:304:CHL:HHB	2.03	0.40
17:N:87:PHE:CD1	17:N:88:LYS:HG3	2.56	0.40
17:N:125:GLY:CA	24:N:312:CHL:HAB	2.48	0.40
25:N:316:CLA:H3A	25:N:316:CLA:HBA2	1.88	0.40
17:8:81:PHE:CE1	17:8:102:LEU:HA	2.56	0.40
18:B:280:PHE:O	18:B:313:ASP:HB2	2.21	0.40
25:B:602:CLA:H18	25:B:602:CLA:H152	1.86	0.40
25:B:615:CLA:H152	25:B:615:CLA:H112	1.87	0.40
19:A:166:GLY:HA3	20:C:346:PHE:HE1	1.85	0.40
20:C:142:LYS:HD3	20:C:249:ARG:HG2	2.04	0.40
25:C:603:CLA:H72	25:C:603:CLA:H112	1.94	0.40
3:h:35:THR:O	3:h:35:THR:OG1	2.32	0.40
17:g:59:TRP:CD1	24:g:313:CHL:HMD3	2.55	0.40
12:u:72:SER:HB2	12:u:78:PHE:CD1	2.56	0.40
12:p:84:LEU:O	12:p:88:HIS:ND1	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:45:THR:HG22	17:q:49:ASN:ND2	2.36	0.40
18:b:198:ILE:HG23	18:b:202:HIS:CE1	2.55	0.40
25:b:608:CLA:C4A	25:b:608:CLA:HBA2	2.50	0.40
25:b:609:CLA:H41	25:b:609:CLA:H61	1.80	0.40
19:a:92:HIS:NE2	20:c:348:ASP:OD2	2.55	0.40
19:a:135:PHE:CE1	20:c:437:ARG:HG3	2.56	0.40
13:s:81:PRO:CD	24:s:402:CHL:HBB1	2.51	0.40
8:r:130:GLU:HB2	24:r:303:CHL:C1B	2.51	0.40
28:r:301:NEX:H11	28:r:301:NEX:H191	1.80	0.40
12:7:167:GLY:HA3	12:7:168:PRO:HD2	1.97	0.40
12:3:145:ILE:HA	12:3:148:ILE:HG22	2.04	0.40
24:3:309:CHL:HAA1	28:3:318:NEX:C25	2.51	0.40
13:S:253:LYS:HD3	25:S:611:CLA:HAA2	2.02	0.40
17:G:130:TYR:CE2	28:G:304:NEX:H191	2.57	0.40
24:9:311:CHL:HMA2	28:9:319:NEX:H30	2.02	0.40
19:A:179:THR:O	19:A:183:MET:HG3	2.22	0.40
20:C:161:TRP:CH2	20:C:226:ILE:HG23	2.55	0.40
20:C:228:ILE:H	20:C:228:ILE:HG12	1.64	0.40
21:D:148:ALA:HB3	21:D:149:PRO:HD3	2.04	0.40
10:4:204:ASP:OD1	10:4:204:ASP:N	2.55	0.40
17:n:62:LEU:HB3	25:n:307:CLA:HBB2	2.02	0.40
28:p:304:NEX:C31	24:p:310:CHL:H3A	2.51	0.40
24:p:305:CHL:HMA3	30:p:319:LHG:H112	2.03	0.40
18:b:53:ASN:HD21	18:b:58:GLN:CD	2.29	0.40
18:b:74:SER:HG	18:b:78:TRP:CG	2.39	0.40
25:c:608:CLA:H111	25:c:608:CLA:H93	1.78	0.40
25:c:609:CLA:H141	25:c:609:CLA:H161	1.89	0.40
21:d:160:TYR:HA	21:d:290:ALA:HB2	2.03	0.40
33:d:411:LMG:H142	33:d:411:LMG:H171	1.47	0.40
26:7:302:0IE:C14	24:7:306:CHL:HMC	2.52	0.40
8:R:179:SER:O	8:R:183:TRP:HD1	2.04	0.40
28:1:303:NEX:H31	28:1:303:NEX:H28	1.98	0.40
11:2:118:TRP:HZ2	24:3:317:CHL:HBD	1.86	0.40
16:T:37:GLU:C	16:T:39:LEU:H	2.30	0.40
17:G:64:THR:HA	17:G:183:PHE:HE2	1.87	0.40
28:G:304:NEX:H31	24:G:310:CHL:HBA1	2.04	0.40
17:N:108:VAL:HG23	24:N:308:CHL:C1D	2.51	0.40
24:N:308:CHL:HHD	24:N:309:CHL:OBD	2.21	0.40
18:B:71:ILE:HD11	25:B:607:CLA:C2A	2.51	0.40
18:B:359:MET:HE2	18:B:366:PHE:H	1.87	0.40
25:B:604:CLA:HMB1	25:B:608:CLA:HHC	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:243:LYS:HB3	20:C:243:LYS:HE2	1.90	0.40
25:C:602:CLA:C1D	25:C:603:CLA:H151	2.51	0.40
21:D:87:HIS:HD2	33:D:401:LMG:HC3	1.86	0.40
17:g:47:ALA:HA	17:g:50:ARG:CZ	2.52	0.40
12:u:186:ASN:ND2	12:u:187:PHE:H	2.20	0.40
25:u:315:CLA:H71	25:u:315:CLA:H111	1.89	0.40
25:u:315:CLA:O2D	25:u:315:CLA:H2A	2.21	0.40
17:y:61:MET:SD	25:y:314:CLA:HAB	2.62	0.40
25:p:317:CLA:HMB1	24:p:318:CHL:HAC2	2.03	0.40
18:b:60:MET:HB3	18:b:60:MET:HE2	1.64	0.40
18:b:115:TRP:NE1	32:b:618:SQD:O8	2.54	0.40
18:b:480:ALA:N	21:d:139:ARG:HH12	2.13	0.40
25:b:607:CLA:H141	25:b:607:CLA:H161	1.83	0.40
19:a:76:ASN:OD1	19:a:76:ASN:N	2.35	0.40
20:c:161:TRP:CH2	20:c:226:ILE:HG23	2.56	0.40
21:d:178:ILE:O	21:d:182:ILE:HG13	2.21	0.40
28:7:304:NEX:C35	24:7:310:CHL:O2A	2.68	0.40
25:7:315:CLA:H2A	25:7:315:CLA:O2D	2.21	0.40
8:R:127:ARG:HA	8:R:127:ARG:HD3	1.99	0.40
25:R:612:CLA:O1D	25:R:612:CLA:H2A	2.22	0.40
10:1:8:ARG:HD2	10:1:31:ASP:O	2.22	0.40
11:2:47:ARG:NH2	11:2:48:ARG:HE	2.20	0.40
11:2:144:LEU:HD23	11:2:144:LEU:HA	1.82	0.40
17:G:134:GLY:HA2	24:G:312:CHL:HAC1	2.02	0.40
12:9:41:ALA:HB1	24:9:304:CHL:HBC1	2.03	0.40
12:9:72:SER:HB2	12:9:78:PHE:CD1	2.56	0.40
17:8:8:ARG:NH2	17:8:24:LEU:O	2.55	0.40
25:B:602:CLA:HED3	25:B:603:CLA:H3A	2.04	0.40
33:B:619:LMG:H291	33:B:619:LMG:H322	1.61	0.40
19:A:82:ILE:HB	19:A:174:LEU:HB2	2.03	0.40
19:A:214:MET:O	19:A:218:LEU:HG	2.22	0.40
30:A:612:LHG:HC12	21:D:269:PHE:CG	2.57	0.40
21:D:152:VAL:HG22	25:D:404:CLA:HED3	2.03	0.40
3:h:13:THR:OG1	25:b:616:CLA:OBD	2.27	0.40
10:4:59:TRP:CE2	24:4:311:CHL:HED2	2.57	0.40
24:g:313:CHL:HHC	24:u:305:CHL:H52	2.03	0.40
12:u:159:CYS:O	12:u:163:ARG:N	2.51	0.40
17:n:39:LEU:HD12	24:n:305:CHL:H11	2.03	0.40
12:p:89:SER:HB2	12:p:205:GLY:CA	2.52	0.40
12:p:142:ALA:HA	24:p:309:CHL:CHC	2.51	0.40
24:p:310:CHL:HMB2	24:p:313:CHL:HMC	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:604:CLA:HMB1	25:b:608:CLA:HHC	2.04	0.40
19:a:159:ILE:C	19:a:162:PRO:HD2	2.47	0.40
19:a:234:ASN:ND2	30:a:601:LHG:O4	2.54	0.40
25:a:604:CLA:H92	25:a:604:CLA:H62	1.80	0.40
21:d:148:ALA:HB3	21:d:149:PRO:HD3	2.04	0.40
25:d:405:CLA:H142	25:d:405:CLA:H112	1.79	0.40
8:r:131:LEU:O	8:r:135:ARG:HG3	2.21	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	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
1	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	E	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	e	63/82 (77%)	63 (100%)	0	0	100	100
3	H	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
3	h	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
4	I	32/36 (89%)	32 (100%)	0	0	100	100
4	i	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
5	K	35/43 (81%)	33 (94%)	2 (6%)	0	100	100
5	k	35/43 (81%)	34 (97%)	1 (3%)	0	100	100
6	L	35/38 (92%)	35 (100%)	0	0	100	100
6	l	35/38 (92%)	35 (100%)	0	0	100	100
7	M	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
7	m	28/33 (85%)	27 (96%)	1 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	R	223/267 (84%)	199 (89%)	23 (10%)	1 (0%)	30	58
8	r	223/267 (84%)	203 (91%)	20 (9%)	0	100	100
9	F	29/42 (69%)	27 (93%)	2 (7%)	0	100	100
9	f	29/42 (69%)	28 (97%)	1 (3%)	0	100	100
10	1	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
10	4	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
11	2	219/256 (86%)	205 (94%)	14 (6%)	0	100	100
11	5	219/256 (86%)	204 (93%)	15 (7%)	0	100	100
12	3	209/254 (82%)	189 (90%)	20 (10%)	0	100	100
12	6	217/254 (85%)	196 (90%)	21 (10%)	0	100	100
12	7	217/254 (85%)	188 (87%)	27 (12%)	2 (1%)	14	41
12	9	217/254 (85%)	185 (85%)	31 (14%)	1 (0%)	24	54
12	p	217/254 (85%)	188 (87%)	26 (12%)	3 (1%)	9	31
12	u	217/254 (85%)	187 (86%)	30 (14%)	0	100	100
13	S	247/308 (80%)	211 (85%)	34 (14%)	2 (1%)	16	44
13	s	247/308 (80%)	209 (85%)	35 (14%)	3 (1%)	10	34
14	X	32/109 (29%)	32 (100%)	0	0	100	100
14	x	32/109 (29%)	32 (100%)	0	0	100	100
15	V	23/33 (70%)	18 (78%)	5 (22%)	0	100	100
15	v	23/33 (70%)	19 (83%)	4 (17%)	0	100	100
16	T	26/31 (84%)	24 (92%)	2 (8%)	0	100	100
16	t	26/31 (84%)	24 (92%)	2 (8%)	0	100	100
17	8	204/280 (73%)	195 (96%)	9 (4%)	0	100	100
17	G	221/280 (79%)	215 (97%)	6 (3%)	0	100	100
17	N	204/280 (73%)	196 (96%)	8 (4%)	0	100	100
17	Y	221/280 (79%)	212 (96%)	9 (4%)	0	100	100
17	g	221/280 (79%)	214 (97%)	7 (3%)	0	100	100
17	n	204/280 (73%)	192 (94%)	11 (5%)	1 (0%)	24	54
17	q	204/280 (73%)	196 (96%)	8 (4%)	0	100	100
17	y	221/280 (79%)	212 (96%)	9 (4%)	0	100	100
18	B	476/508 (94%)	455 (96%)	19 (4%)	2 (0%)	30	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	b	476/508 (94%)	457 (96%)	17 (4%)	2 (0%)	30	58
19	A	325/327 (99%)	307 (94%)	17 (5%)	1 (0%)	36	64
19	a	325/327 (99%)	304 (94%)	20 (6%)	1 (0%)	36	64
20	C	446/461 (97%)	409 (92%)	36 (8%)	1 (0%)	43	71
20	c	446/461 (97%)	407 (91%)	38 (8%)	1 (0%)	43	71
21	D	338/352 (96%)	313 (93%)	25 (7%)	0	100	100
21	d	338/352 (96%)	318 (94%)	20 (6%)	0	100	100
22	W	41/118 (35%)	30 (73%)	11 (27%)	0	100	100
22	w	41/118 (35%)	30 (73%)	11 (27%)	0	100	100
All	All	8900/10550 (84%)	8243 (93%)	636 (7%)	21 (0%)	44	71

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	B	279	PHE
18	B	299	SER
17	n	23	TYR
12	p	117	VAL
12	p	118	TRP
12	p	186	ASN
18	b	279	PHE
18	b	299	SER
12	7	117	VAL
12	7	118	TRP
13	S	163	LEU
20	C	449	ARG
20	c	449	ARG
13	s	163	LEU
8	R	42	SER
19	A	141	PRO
19	a	141	PRO
13	s	59	PHE
13	S	173	VAL
13	s	173	VAL
12	9	117	VAL

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	Z	51/52 (98%)	51 (100%)	0	100	100
1	z	51/52 (98%)	51 (100%)	0	100	100
2	E	58/73 (80%)	57 (98%)	1 (2%)	53	71
2	e	58/73 (80%)	57 (98%)	1 (2%)	53	71
3	H	56/62 (90%)	55 (98%)	1 (2%)	51	70
3	h	56/62 (90%)	55 (98%)	1 (2%)	51	70
4	I	31/32 (97%)	31 (100%)	0	100	100
4	i	31/32 (97%)	31 (100%)	0	100	100
5	K	33/39 (85%)	31 (94%)	2 (6%)	17	44
5	k	33/39 (85%)	32 (97%)	1 (3%)	36	62
6	L	34/35 (97%)	31 (91%)	3 (9%)	9	31
6	l	34/35 (97%)	32 (94%)	2 (6%)	18	45
7	M	27/30 (90%)	27 (100%)	0	100	100
7	m	27/30 (90%)	26 (96%)	1 (4%)	30	58
8	R	181/214 (85%)	173 (96%)	8 (4%)	25	54
8	r	180/214 (84%)	170 (94%)	10 (6%)	19	46
9	F	25/36 (69%)	22 (88%)	3 (12%)	5	19
9	f	26/36 (72%)	23 (88%)	3 (12%)	5	21
10	1	160/160 (100%)	153 (96%)	7 (4%)	25	54
10	4	159/160 (99%)	153 (96%)	6 (4%)	29	57
11	2	168/199 (84%)	168 (100%)	0	100	100
11	5	168/199 (84%)	168 (100%)	0	100	100
12	3	165/202 (82%)	158 (96%)	7 (4%)	26	55
12	6	172/202 (85%)	166 (96%)	6 (4%)	32	59
12	7	173/202 (86%)	164 (95%)	9 (5%)	21	49
12	9	174/202 (86%)	167 (96%)	7 (4%)	28	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	p	174/202 (86%)	161 (92%)	13 (8%)	12	37
12	u	175/202 (87%)	166 (95%)	9 (5%)	21	50
13	S	184/232 (79%)	172 (94%)	12 (6%)	15	42
13	s	184/232 (79%)	174 (95%)	10 (5%)	20	48
14	X	24/80 (30%)	23 (96%)	1 (4%)	26	55
14	x	24/80 (30%)	22 (92%)	2 (8%)	10	33
15	V	20/28 (71%)	18 (90%)	2 (10%)	7	26
15	v	20/28 (71%)	19 (95%)	1 (5%)	22	50
16	T	25/28 (89%)	23 (92%)	2 (8%)	11	35
16	t	25/28 (89%)	23 (92%)	2 (8%)	11	35
17	8	153/210 (73%)	152 (99%)	1 (1%)	76	80
17	G	165/210 (79%)	161 (98%)	4 (2%)	43	66
17	N	152/210 (72%)	143 (94%)	9 (6%)	18	45
17	Y	165/210 (79%)	162 (98%)	3 (2%)	51	70
17	g	165/210 (79%)	159 (96%)	6 (4%)	31	58
17	n	151/210 (72%)	144 (95%)	7 (5%)	24	53
17	q	153/210 (73%)	153 (100%)	0	100	100
17	y	165/210 (79%)	163 (99%)	2 (1%)	63	75
18	B	384/410 (94%)	371 (97%)	13 (3%)	32	60
18	b	384/410 (94%)	372 (97%)	12 (3%)	35	61
19	A	266/266 (100%)	251 (94%)	15 (6%)	19	46
19	a	266/266 (100%)	252 (95%)	14 (5%)	20	48
20	C	347/359 (97%)	338 (97%)	9 (3%)	40	65
20	c	347/359 (97%)	337 (97%)	10 (3%)	37	63
21	D	275/285 (96%)	266 (97%)	9 (3%)	33	60
21	d	275/285 (96%)	267 (97%)	8 (3%)	37	63
22	W	29/88 (33%)	27 (93%)	2 (7%)	14	40
22	w	29/88 (33%)	29 (100%)	0	100	100
All	All	7057/8308 (85%)	6800 (96%)	257 (4%)	32	58

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	75	VAL
3	H	12	VAL
5	K	24	ILE
5	K	40	VAL
6	L	12	GLU
6	L	14	ASN
6	L	16	THR
8	R	48	MET
8	R	76	VAL
8	R	153	VAL
8	R	156	GLN
8	R	164	GLN
8	R	182	VAL
8	R	202	THR
8	R	261	LEU
9	F	15	VAL
9	F	16	ARG
9	F	42	ARG
10	1	1	VAL
10	1	8	ARG
10	1	12	LEU
10	1	52	LEU
10	1	69	THR
10	1	85	VAL
10	1	188	LEU
12	3	52	VAL
12	3	101	THR
12	3	207	LEU
12	3	218	GLN
12	3	221	VAL
12	3	240	ASN
12	3	241	ASN
13	S	61	GLU
13	S	84	LEU
13	S	86	ASP
13	S	119	LEU
13	S	124	LEU
13	S	128	ARG
13	S	150	LEU
13	S	164	ASN
13	S	168	LEU
13	S	171	PHE
13	S	193	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	S	271	GLN
14	X	90	LEU
15	V	282	GLN
15	V	298	VAL
16	T	40	VAL
16	T	55	SER
17	G	20	VAL
17	G	54	LEU
17	G	69	THR
17	G	108	VAL
12	9	44	LEU
12	9	100	LEU
12	9	101	THR
12	9	117	VAL
12	9	239	ASN
12	9	248	ILE
12	9	250	ARG
17	N	12	LEU
17	N	20	VAL
17	N	54	LEU
17	N	62	LEU
17	N	65	VAL
17	N	68	LEU
17	N	69	THR
17	N	107	LEU
17	N	108	VAL
17	Y	16	SER
17	Y	73	LEU
17	Y	180	MET
17	8	1	VAL
18	B	10	THR
18	B	12	VAL
18	B	15	ASP
18	B	41	GLU
18	B	52	LEU
18	B	158	VAL
18	B	224	ARG
18	B	237	VAL
18	B	276	ASP
18	B	280	PHE
18	B	365	THR
18	B	368	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	B	431	GLU
19	A	28	LEU
19	A	60	ILE
19	A	76	ASN
19	A	85	THR
19	A	121	LEU
19	A	140	ARG
19	A	143	ILE
19	A	223	LEU
19	A	232	SER
19	A	245	THR
19	A	249	VAL
19	A	281	VAL
19	A	313	VAL
19	A	322	ASN
19	A	326	LEU
20	C	129	GLU
20	C	213	VAL
20	C	222	ILE
20	C	228	ILE
20	C	343	THR
20	C	357	LEU
20	C	389	LEU
20	C	395	VAL
20	C	405	VAL
21	D	28	VAL
21	D	89	LEU
21	D	102	THR
21	D	192	THR
21	D	213	ILE
21	D	279	LEU
21	D	329	MET
21	D	340	VAL
21	D	345	VAL
22	W	84	LEU
22	W	96	TRP
2	e	75	VAL
3	h	18	LEU
5	k	40	VAL
6	l	12	GLU
6	l	16	THR
7	m	3	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	f	15	VAL
9	f	16	ARG
9	f	42	ARG
10	4	10	LEU
10	4	12	LEU
10	4	52	LEU
10	4	69	THR
10	4	85	VAL
10	4	188	LEU
12	6	48	SER
12	6	52	VAL
12	6	101	THR
12	6	108	TYR
12	6	234	ILE
12	6	240	ASN
14	x	79	LEU
14	x	90	LEU
15	v	298	VAL
16	t	40	VAL
16	t	55	SER
17	g	1	VAL
17	g	20	VAL
17	g	25	THR
17	g	69	THR
17	g	108	VAL
17	g	123	LEU
12	u	44	LEU
12	u	101	THR
12	u	111	VAL
12	u	117	VAL
12	u	207	LEU
12	u	242	ILE
12	u	248	ILE
12	u	249	THR
12	u	250	ARG
17	n	12	LEU
17	n	20	VAL
17	n	24	LEU
17	n	54	LEU
17	n	62	LEU
17	n	68	LEU
17	n	102	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	y	10	LEU
17	y	73	LEU
12	p	48	SER
12	p	80	GLN
12	p	96	THR
12	p	101	THR
12	p	111	VAL
12	p	113	LEU
12	p	117	VAL
12	p	119	PHE
12	p	145	ILE
12	p	221	VAL
12	p	239	ASN
12	p	245	ASP
12	p	249	THR
18	b	10	THR
18	b	12	VAL
18	b	15	ASP
18	b	41	GLU
18	b	52	LEU
18	b	57	ARG
18	b	60	MET
18	b	237	VAL
18	b	276	ASP
18	b	365	THR
18	b	368	VAL
18	b	431	GLU
19	a	28	LEU
19	a	60	ILE
19	a	76	ASN
19	a	85	THR
19	a	102	LEU
19	a	121	LEU
19	a	140	ARG
19	a	143	ILE
19	a	223	LEU
19	a	245	THR
19	a	249	VAL
19	a	281	VAL
19	a	322	ASN
19	a	326	LEU
20	c	129	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	c	213	VAL
20	c	222	ILE
20	c	228	ILE
20	c	343	THR
20	c	357	LEU
20	c	389	LEU
20	c	392	LEU
20	c	393	ASN
20	c	405	VAL
21	d	89	LEU
21	d	102	THR
21	d	192	THR
21	d	213	ILE
21	d	279	LEU
21	d	329	MET
21	d	340	VAL
21	d	345	VAL
13	s	61	GLU
13	s	84	LEU
13	s	86	ASP
13	s	119	LEU
13	s	124	LEU
13	s	164	ASN
13	s	168	LEU
13	s	171	PHE
13	s	193	VAL
13	s	271	GLN
8	r	48	MET
8	r	76	VAL
8	r	81	PHE
8	r	82	ASP
8	r	153	VAL
8	r	156	GLN
8	r	164	GLN
8	r	182	VAL
8	r	202	THR
8	r	261	LEU
12	7	42	LEU
12	7	48	SER
12	7	80	GLN
12	7	96	THR
12	7	111	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	7	117	VAL
12	7	145	ILE
12	7	186	ASN
12	7	247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	100	ASN
2	E	104	GLN
4	I	31	ASN
4	I	34	GLN
8	R	80	GLN
8	R	89	ASN
10	1	186	GLN
11	2	133	ASN
11	2	189	GLN
11	2	215	GLN
12	3	241	ASN
13	S	65	GLN
13	S	180	ASN
12	9	141	HIS
12	9	143	GLN
12	9	229	ASN
12	9	239	ASN
17	N	104	ASN
17	N	111	GLN
18	B	26	HIS
18	B	53	ASN
18	B	58	GLN
18	B	331	ASN
18	B	425	GLN
19	A	26	ASN
19	A	261	GLN
19	A	315	ASN
20	C	366	ASN
20	C	451	ASN
21	D	197	HIS
21	D	230	ASN
1	z	6	GLN
2	e	100	ASN
4	i	31	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	i	34	GLN
11	5	215	GLN
17	g	104	ASN
12	u	141	HIS
12	u	143	GLN
17	n	189	GLN
17	q	92	GLN
18	b	26	HIS
18	b	53	ASN
18	b	58	GLN
18	b	331	ASN
18	b	425	GLN
19	a	26	ASN
19	a	75	ASN
19	a	241	GLN
19	a	315	ASN
20	c	366	ASN
20	c	451	ASN
13	s	248	GLN
8	r	216	ASN
12	7	81	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 528 ligands modelled in this entry, 2 are monoatomic - leaving 526 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	$\#\|Z\| > 2$
24	CHL	G	313	-	70,74,74	1.98	18 (25%)	80,114,114	2.74	29 (36%)
25	CLA	1	307	-	45,49,73	1.52	9 (20%)	54,84,113	1.49	6 (11%)
25	CLA	G	314	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
25	CLA	y	316	17	49,53,73	1.48	10 (20%)	59,89,113	1.53	4 (6%)
24	CHL	2	310	-	46,50,74	2.30	19 (41%)	51,85,114	3.39	24 (47%)
25	CLA	7	316	12	49,53,73	1.47	10 (20%)	59,89,113	1.45	4 (6%)
26	0IE	G	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.55	9 (18%)
24	CHL	4	310	-	47,51,74	2.24	18 (38%)	52,86,114	3.32	25 (48%)
29	0UR	u	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.79	13 (22%)
24	CHL	q	308	-	50,54,74	2.21	18 (36%)	56,90,114	3.33	28 (50%)
30	LHG	d	407	-	48,48,48	1.07	5 (10%)	51,54,54	0.96	2 (3%)
31	8CT	S	614	-	40,41,41	4.72	24 (60%)	50,56,56	2.96	18 (36%)
25	CLA	R	609	8	59,63,73	1.34	9 (15%)	71,101,113	1.36	6 (8%)
24	CHL	R	606	-	52,56,74	2.18	18 (34%)	58,92,114	3.23	25 (43%)
26	0IE	R	614	-	42,45,45	1.44	6 (14%)	49,63,63	1.54	10 (20%)
30	LHG	G	319	-	42,42,48	1.16	6 (14%)	45,48,54	0.99	2 (4%)
25	CLA	C	609	20	69,73,73	1.26	9 (13%)	83,113,113	1.36	8 (9%)
30	LHG	9	318	25	42,42,48	1.17	6 (14%)	45,48,54	0.98	2 (4%)
24	CHL	q	304	17	64,68,74	1.96	19 (29%)	72,106,114	2.92	30 (41%)
25	CLA	4	314	-	45,49,73	1.52	9 (20%)	54,84,113	1.51	5 (9%)
30	LHG	5	319	-	42,42,48	1.16	5 (11%)	45,48,54	1.04	4 (8%)
25	CLA	3	316	-	49,53,73	1.49	10 (20%)	59,89,113	1.46	7 (11%)
25	CLA	7	308	-	54,58,73	1.40	9 (16%)	65,95,113	1.40	5 (7%)
37	DGD	C	619	-	51,51,67	0.93	2 (3%)	65,65,81	1.24	5 (7%)
25	CLA	s	413	-	59,63,73	1.34	10 (16%)	70,100,113	1.39	6 (8%)
31	8CT	d	410	-	40,41,41	4.69	23 (57%)	50,56,56	2.50	17 (34%)
24	CHL	2	305	11	48,52,74	2.21	17 (35%)	53,87,114	3.32	23 (43%)
25	CLA	Y	306	17	57,61,73	1.37	9 (15%)	68,98,113	1.40	6 (8%)
25	CLA	3	307	-	47,51,73	1.48	8 (17%)	56,86,113	1.46	4 (7%)
25	CLA	4	306	-	48,52,73	1.47	8 (16%)	56,87,113	1.46	6 (10%)
25	CLA	6	313	-	45,49,73	1.52	7 (15%)	54,84,113	1.52	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	s	408	-	50,54,74	2.19	19 (38%)	56,90,114	3.32	24 (42%)
25	CLA	C	608	20	65,69,73	1.28	10 (15%)	78,108,113	1.38	8 (10%)
24	CHL	1	308	10	47,51,74	2.33	18 (38%)	52,86,114	3.37	24 (46%)
36	BCT	A	611	38	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
24	CHL	G	309	-	47,51,74	2.36	18 (38%)	52,86,114	3.36	24 (46%)
25	CLA	g	317	17	59,63,73	1.35	9 (15%)	70,100,113	1.37	7 (10%)
25	CLA	u	314	-	59,63,73	1.35	7 (11%)	71,101,113	1.35	7 (9%)
25	CLA	r	305	-	45,49,73	1.52	10 (22%)	54,84,113	1.56	7 (12%)
25	CLA	y	314	17	59,63,73	1.34	10 (16%)	71,101,113	1.37	8 (11%)
30	LHG	A	612	-	43,43,48	1.15	5 (11%)	46,49,54	1.02	3 (6%)
24	CHL	2	318	11	46,50,74	2.37	18 (39%)	51,85,114	3.41	25 (49%)
30	LHG	C	617	-	31,31,48	1.31	5 (16%)	34,37,54	1.14	3 (8%)
25	CLA	9	316	12	59,63,73	1.36	9 (15%)	70,100,113	1.34	6 (8%)
24	CHL	g	306	-	68,72,74	1.91	19 (27%)	77,111,114	2.88	30 (38%)
24	CHL	u	318	-	46,50,74	2.43	19 (41%)	51,85,114	3.45	26 (50%)
24	CHL	Y	312	-	70,74,74	1.88	19 (27%)	80,114,114	2.77	27 (33%)
24	CHL	1	311	-	48,52,74	2.20	18 (37%)	53,87,114	3.29	24 (45%)
24	CHL	y	310	-	51,55,74	2.14	19 (37%)	57,91,114	3.31	28 (49%)
25	CLA	C	602	20	69,73,73	1.25	10 (14%)	83,113,113	1.32	6 (7%)
24	CHL	5	305	11	48,52,74	2.21	17 (35%)	53,87,114	3.33	24 (45%)
25	CLA	B	606	18	69,73,73	1.24	9 (13%)	83,113,113	1.36	8 (9%)
25	CLA	A	604	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
28	NEX	N	303	-	38,46,46	1.05	2 (5%)	50,70,70	2.82	17 (34%)
25	CLA	B	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
25	CLA	n	306	17	58,62,73	1.37	8 (13%)	69,99,113	1.38	6 (8%)
24	CHL	S	607	-	50,54,74	2.20	19 (38%)	56,90,114	3.30	24 (42%)
32	SQD	D	409	-	43,44,54	1.06	5 (11%)	52,55,65	1.57	9 (17%)
24	CHL	q	303	17	58,62,74	2.13	18 (31%)	65,99,114	3.05	27 (41%)
25	CLA	6	306	-	45,49,73	1.50	9 (20%)	54,84,113	1.51	6 (11%)
24	CHL	r	309	-	50,54,74	2.24	18 (36%)	56,90,114	3.21	27 (48%)
25	CLA	s	410	-	59,63,73	1.33	10 (16%)	71,101,113	1.35	5 (7%)
25	CLA	R	613	-	51,55,73	1.46	8 (15%)	61,91,113	1.37	5 (8%)
31	8CT	s	415	-	40,41,41	4.72	24 (60%)	50,56,56	2.97	18 (36%)
25	CLA	B	608	-	59,63,73	1.35	10 (16%)	71,101,113	1.36	7 (9%)
31	8CT	V	401	-	40,41,41	4.66	23 (57%)	50,56,56	2.56	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	R	612	-	49,53,73	1.49	8 (16%)	59,89,113	1.48	6 (10%)
24	CHL	u	309	12	47,51,74	2.34	18 (38%)	52,86,114	3.34	24 (46%)
28	NEX	p	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
29	0UR	g	301	-	50,53,58	0.95	1 (2%)	58,72,77	1.73	16 (27%)
25	CLA	3	313	-	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
24	CHL	S	605	-	50,54,74	2.23	18 (36%)	56,90,114	3.24	23 (41%)
23	HEM	f	201	2,9	50,50,50	1.37	7 (14%)	66,82,82	1.09	3 (4%)
25	CLA	2	316	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
24	CHL	p	305	12	70,74,74	1.82	19 (27%)	80,114,114	2.88	31 (38%)
24	CHL	q	311	-	60,64,74	2.02	19 (31%)	68,102,114	3.00	28 (41%)
25	CLA	A	610	-	45,49,73	1.52	8 (17%)	54,84,113	1.53	7 (12%)
24	CHL	u	306	-	68,72,74	1.95	19 (27%)	77,111,114	2.81	27 (35%)
24	CHL	1	317	-	46,50,74	2.41	19 (41%)	51,85,114	3.40	25 (49%)
30	LHG	n	318	-	42,42,48	1.18	6 (14%)	45,48,54	0.97	2 (4%)
24	CHL	2	313	-	46,50,74	2.33	18 (39%)	51,85,114	3.34	25 (49%)
25	CLA	D	405	21	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
24	CHL	y	311	-	58,62,74	2.04	19 (32%)	65,99,114	3.18	31 (47%)
24	CHL	N	304	17	58,62,74	2.15	18 (31%)	65,99,114	3.04	27 (41%)
24	CHL	S	613	-	46,50,74	2.29	18 (39%)	51,85,114	3.43	27 (52%)
30	LHG	7	319	25	36,36,48	1.25	5 (13%)	39,42,54	1.08	2 (5%)
26	0IE	7	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.60	12 (24%)
24	CHL	9	311	-	51,55,74	2.24	19 (37%)	57,91,114	3.22	25 (43%)
25	CLA	9	307	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	5 (7%)
25	CLA	A	607	19	64,68,73	1.27	9 (14%)	77,107,113	1.41	8 (10%)
26	0IE	g	303	-	42,45,45	1.41	6 (14%)	49,63,63	1.54	9 (18%)
25	CLA	y	307	17	57,61,73	1.37	9 (15%)	68,98,113	1.41	7 (10%)
25	CLA	C	605	20	60,64,73	1.32	10 (16%)	72,102,113	1.40	7 (9%)
28	NEX	g	304	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	R	611	8	49,53,73	1.48	10 (20%)	59,89,113	1.45	5 (8%)
24	CHL	N	309	-	50,54,74	2.18	18 (36%)	56,90,114	3.34	28 (50%)
24	CHL	S	601	13	50,54,74	2.18	19 (38%)	56,90,114	3.35	24 (42%)
24	CHL	n	308	17	47,51,74	2.30	18 (38%)	52,86,114	3.32	24 (46%)
31	8CT	v	401	-	40,41,41	4.67	23 (57%)	50,56,56	2.55	17 (34%)
25	CLA	3	306	-	45,49,73	1.52	9 (20%)	54,84,113	1.51	5 (9%)
25	CLA	b	604	18	66,70,73	1.27	9 (13%)	79,109,113	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	C	611	20	69,73,73	1.25	11 (15%)	83,113,113	1.34	5 (6%)
26	0IE	5	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.53	9 (18%)
24	CHL	7	312	-	51,55,74	2.09	18 (35%)	57,91,114	3.34	28 (49%)
25	CLA	n	307	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	7 (10%)
24	CHL	4	308	10	47,51,74	2.33	18 (38%)	52,86,114	3.37	24 (46%)
25	CLA	9	313	-	59,63,73	1.35	7 (11%)	71,101,113	1.36	7 (9%)
25	CLA	C	607	-	69,73,73	1.23	11 (15%)	83,113,113	1.33	5 (6%)
24	CHL	n	312	-	60,64,74	2.06	18 (30%)	68,102,114	2.99	28 (41%)
25	CLA	r	311	-	49,53,73	1.47	8 (16%)	59,89,113	1.46	7 (11%)
26	0IE	1	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.57	10 (20%)
25	CLA	B	602	18	69,73,73	1.24	10 (14%)	83,113,113	1.30	6 (7%)
33	LMG	w	201	-	36,36,55	1.05	2 (5%)	44,44,63	1.35	6 (13%)
24	CHL	9	317	-	46,50,74	2.43	19 (41%)	51,85,114	3.46	26 (50%)
26	0IE	6	302	-	41,44,45	1.45	6 (14%)	46,60,63	1.67	11 (23%)
37	DGD	c	618	-	51,51,67	0.93	2 (3%)	65,65,81	1.22	6 (9%)
25	CLA	7	315	30	67,71,73	1.25	10 (14%)	80,110,113	1.38	7 (8%)
25	CLA	N	314	-	67,71,73	1.26	8 (11%)	80,110,113	1.29	5 (6%)
25	CLA	C	604	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
24	CHL	y	312	-	55,59,74	2.07	18 (32%)	62,96,114	3.16	29 (46%)
30	LHG	y	319	25	42,42,48	1.15	5 (11%)	45,48,54	1.07	2 (4%)
30	LHG	D	407	-	48,48,48	1.08	5 (10%)	51,54,54	0.96	2 (3%)
25	CLA	g	314	-	59,63,73	1.35	9 (15%)	71,101,113	1.35	7 (9%)
25	CLA	b	614	18	60,64,73	1.33	10 (16%)	72,102,113	1.35	4 (5%)
24	CHL	N	310	-	57,61,74	2.17	18 (31%)	64,98,114	3.11	28 (43%)
25	CLA	5	307	11	47,51,73	1.48	9 (19%)	56,86,113	1.46	5 (8%)
24	CHL	2	306	-	51,55,74	2.17	19 (37%)	57,91,114	3.20	25 (43%)
24	CHL	p	311	-	50,54,74	2.26	19 (38%)	56,90,114	3.19	24 (42%)
25	CLA	c	608	20	65,69,73	1.28	9 (13%)	78,108,113	1.38	8 (10%)
24	CHL	9	308	12	47,51,74	2.36	18 (38%)	52,86,114	3.36	25 (48%)
25	CLA	u	315	-	67,71,73	1.28	7 (10%)	80,110,113	1.32	6 (7%)
29	0UR	9	301	-	50,53,58	0.93	1 (2%)	58,72,77	1.76	13 (22%)
26	0IE	y	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.54	10 (20%)
24	CHL	3	311	-	48,52,74	2.20	18 (37%)	53,87,114	3.36	25 (47%)
24	CHL	r	303	-	51,55,74	2.16	18 (35%)	57,91,114	3.25	26 (45%)
24	CHL	4	317	-	46,50,74	2.41	19 (41%)	51,85,114	3.41	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	y	315	30	67,71,73	1.25	9 (13%)	80,110,113	1.28	5 (6%)
25	CLA	G	307	-	57,61,73	1.39	8 (14%)	68,98,113	1.34	5 (7%)
25	CLA	8	311	-	59,63,73	1.33	10 (16%)	71,101,113	1.38	7 (9%)
24	CHL	y	305	17	70,74,74	1.80	18 (25%)	80,114,114	2.87	29 (36%)
24	CHL	7	305	12	70,74,74	1.82	18 (25%)	80,114,114	2.88	31 (38%)
25	CLA	G	317	-	59,63,73	1.34	9 (15%)	70,100,113	1.37	7 (10%)
24	CHL	r	308	-	52,56,74	2.13	19 (36%)	58,92,114	3.31	27 (46%)
25	CLA	b	605	18	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
29	0UR	6	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.81	14 (24%)
25	CLA	r	312	8	49,53,73	1.48	10 (20%)	59,89,113	1.45	5 (8%)
26	0IE	3	302	-	41,44,45	1.44	6 (14%)	46,60,63	1.65	11 (23%)
25	CLA	C	612	20	58,62,73	1.34	10 (17%)	69,99,113	1.43	5 (7%)
24	CHL	g	311	-	58,62,74	2.14	18 (31%)	65,99,114	3.06	27 (41%)
28	NEX	s	401	25	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
24	CHL	N	311	-	54,58,74	2.14	19 (35%)	59,94,114	3.20	25 (42%)
25	CLA	1	316	10	46,50,73	1.51	7 (15%)	55,85,113	1.47	5 (9%)
28	NEX	u	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
26	0IE	G	302	-	42,45,45	1.42	6 (14%)	49,63,63	1.58	9 (18%)
25	CLA	5	315	-	67,71,73	1.26	9 (13%)	80,110,113	1.31	5 (6%)
24	CHL	Y	305	-	68,72,74	1.85	18 (26%)	77,111,114	2.92	29 (37%)
26	0IE	u	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.53	11 (22%)
24	CHL	n	317	-	46,50,74	2.42	19 (41%)	51,85,114	3.45	26 (50%)
32	SQD	b	618	-	53,54,54	0.96	5 (9%)	62,65,65	1.55	11 (17%)
24	CHL	8	309	-	54,58,74	2.08	18 (33%)	59,94,114	3.19	26 (44%)
25	CLA	s	412	13	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
25	CLA	b	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
25	CLA	b	609	18	69,73,73	1.24	9 (13%)	83,113,113	1.32	8 (9%)
26	0IE	n	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.58	11 (22%)
24	CHL	8	315	-	46,50,74	2.39	19 (41%)	51,85,114	3.42	25 (49%)
25	CLA	c	604	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
25	CLA	a	607	19	64,68,73	1.28	9 (14%)	77,107,113	1.42	9 (11%)
30	LHG	a	612	-	43,43,48	1.15	5 (11%)	46,49,54	1.02	3 (6%)
24	CHL	6	311	-	48,52,74	2.18	18 (37%)	53,87,114	3.36	25 (47%)
25	CLA	5	314	-	59,63,73	1.34	10 (16%)	71,101,113	1.35	6 (8%)
26	0IE	4	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.58	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	612	18	69,73,73	1.24	10 (14%)	83,113,113	1.35	9 (10%)
29	0UR	2	301	-	50,53,58	1.00	2 (4%)	58,72,77	1.84	15 (25%)
24	CHL	S	602	13	62,66,74	1.97	18 (29%)	70,104,114	2.98	28 (40%)
24	CHL	N	308	17	47,51,74	2.27	17 (36%)	52,86,114	3.30	24 (46%)
24	CHL	G	318	17	46,50,74	2.32	18 (39%)	51,85,114	3.42	25 (49%)
25	CLA	u	316	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	4 (6%)
25	CLA	a	604	-	69,73,73	1.27	10 (14%)	83,113,113	1.30	7 (8%)
25	CLA	1	314	-	45,49,73	1.52	8 (17%)	54,84,113	1.51	5 (9%)
25	CLA	N	316	-	47,51,73	1.49	9 (19%)	56,86,113	1.41	4 (7%)
26	0IE	9	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.58	10 (20%)
25	CLA	Y	315	17	49,53,73	1.47	10 (20%)	59,89,113	1.53	4 (6%)
29	0UR	3	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.71	12 (20%)
24	CHL	3	305	-	52,56,74	2.21	19 (36%)	58,92,114	3.15	25 (43%)
25	CLA	r	313	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	7 (11%)
25	CLA	c	611	20	69,73,73	1.24	11 (15%)	83,113,113	1.32	5 (6%)
24	CHL	Y	311	-	55,59,74	2.08	18 (32%)	62,96,114	3.16	29 (46%)
28	NEX	R	616	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	S	610	-	49,53,73	1.47	10 (20%)	59,89,113	1.43	5 (8%)
25	CLA	1	313	-	59,63,73	1.35	8 (13%)	71,101,113	1.36	7 (9%)
24	CHL	9	312	-	47,51,74	2.33	17 (36%)	52,86,114	3.31	25 (48%)
25	CLA	5	308	-	54,58,73	1.39	8 (14%)	65,95,113	1.44	8 (12%)
25	CLA	c	612	20	58,62,73	1.34	10 (17%)	69,99,113	1.42	4 (5%)
31	8CT	A	608	-	40,41,41	4.63	23 (57%)	50,56,56	2.65	20 (40%)
24	CHL	1	305	10	50,54,74	2.23	19 (38%)	56,90,114	3.29	28 (50%)
25	CLA	C	606	20	57,61,73	1.37	10 (17%)	68,98,113	1.41	6 (8%)
24	CHL	G	306	17	68,72,74	1.92	19 (27%)	77,111,114	2.86	29 (37%)
25	CLA	q	314	17	49,53,73	1.48	8 (16%)	59,89,113	1.48	4 (6%)
25	CLA	G	316	17	49,53,73	1.49	10 (20%)	59,89,113	1.46	4 (6%)
24	CHL	6	309	-	55,59,74	2.19	18 (32%)	62,96,114	3.12	28 (45%)
24	CHL	s	402	13	50,54,74	2.19	19 (38%)	56,90,114	3.35	24 (42%)
24	CHL	2	312	-	50,54,74	2.20	19 (38%)	56,90,114	3.27	25 (44%)
33	LMG	d	401	-	48,48,55	0.91	2 (4%)	56,56,63	1.19	5 (8%)
25	CLA	B	612	18	69,73,73	1.23	10 (14%)	83,113,113	1.36	8 (9%)
24	CHL	4	309	-	47,51,74	2.31	17 (36%)	52,86,114	3.29	25 (48%)
24	CHL	R	608	-	50,54,74	2.25	18 (36%)	56,90,114	3.21	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	6	310	-	50,54,74	2.34	18 (36%)	56,90,114	3.20	24 (42%)
25	CLA	R	604	-	45,49,73	1.51	10 (22%)	54,84,113	1.55	8 (14%)
25	CLA	n	316	-	47,51,73	1.49	7 (14%)	56,86,113	1.41	4 (7%)
26	0IE	N	302	-	42,45,45	1.42	6 (14%)	49,63,63	1.58	11 (22%)
25	CLA	c	605	20	60,64,73	1.32	10 (16%)	72,102,113	1.39	6 (8%)
24	CHL	N	317	-	46,50,74	2.41	19 (41%)	51,85,114	3.45	26 (50%)
25	CLA	4	316	-	46,50,73	1.52	7 (15%)	55,85,113	1.46	5 (9%)
24	CHL	5	306	-	51,55,74	2.17	19 (37%)	57,91,114	3.20	25 (43%)
25	CLA	s	417	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)
27	XAT	r	316	-	39,47,47	0.92	0	54,74,74	2.72	19 (35%)
26	0IE	2	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.52	9 (18%)
24	CHL	5	312	-	50,54,74	2.20	19 (38%)	56,90,114	3.27	24 (42%)
33	LMG	D	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.13	4 (7%)
24	CHL	y	318	17	46,50,74	2.26	18 (39%)	51,85,114	3.43	27 (52%)
25	CLA	8	312	-	67,71,73	1.26	9 (13%)	80,110,113	1.29	6 (7%)
26	0IE	p	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.57	9 (18%)
24	CHL	2	311	-	51,55,74	2.26	19 (37%)	57,91,114	3.14	25 (43%)
26	0IE	Y	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.55	10 (20%)
24	CHL	g	312	-	55,59,74	2.17	19 (34%)	62,96,114	3.11	29 (46%)
24	CHL	q	307	17	47,51,74	2.24	18 (38%)	52,86,114	3.34	24 (46%)
26	0IE	q	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.52	10 (20%)
25	CLA	B	615	18	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
25	CLA	R	610	-	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
25	CLA	5	317	11	53,57,73	1.39	9 (16%)	62,93,113	1.45	6 (9%)
25	CLA	3	314	-	45,49,73	1.51	7 (15%)	54,84,113	1.47	7 (12%)
31	8CT	t	101	-	40,41,41	4.64	23 (57%)	50,56,56	3.04	18 (36%)
24	CHL	7	313	-	47,51,74	2.22	18 (38%)	52,86,114	3.30	23 (44%)
25	CLA	b	607	18	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
29	0UR	N	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.82	12 (20%)
31	8CT	C	613	-	40,41,41	4.60	23 (57%)	50,56,56	2.72	20 (40%)
25	CLA	p	308	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	5 (7%)
31	8CT	S	615	-	40,41,41	4.73	25 (62%)	50,56,56	7.31	22 (44%)
24	CHL	4	304	-	46,50,74	2.40	19 (41%)	51,85,114	3.38	26 (50%)
24	CHL	q	310	-	54,58,74	2.09	18 (33%)	59,94,114	3.18	26 (44%)
24	CHL	s	403	13	62,66,74	1.97	18 (29%)	70,104,114	2.97	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	p	317	12	59,63,73	1.34	10 (16%)	70,100,113	1.39	6 (8%)
25	CLA	n	313	-	59,63,73	1.34	8 (13%)	71,101,113	1.36	7 (9%)
24	CHL	3	309	-	55,59,74	2.20	18 (32%)	62,96,114	3.12	28 (45%)
25	CLA	7	317	12	56,60,73	1.38	10 (17%)	67,97,113	1.42	6 (8%)
25	CLA	C	601	20	69,73,73	1.24	10 (14%)	83,113,113	1.37	8 (9%)
24	CHL	r	306	-	46,50,74	2.32	19 (41%)	51,85,114	3.36	25 (49%)
24	CHL	u	312	-	51,55,74	2.24	18 (35%)	57,91,114	3.22	24 (42%)
24	CHL	8	310	-	60,64,74	2.03	19 (31%)	68,102,114	3.00	27 (39%)
24	CHL	Y	319	-	57,61,74	2.09	18 (31%)	64,98,114	3.15	30 (46%)
25	CLA	c	616	20	50,54,73	1.43	10 (20%)	60,90,113	1.49	7 (11%)
36	BCT	a	611	38	2,3,3	1.25	0	2,3,3	4.16	2 (100%)
29	0UR	5	301	-	50,53,58	0.99	2 (4%)	58,72,77	1.84	15 (25%)
29	0UR	Y	301	-	50,53,58	0.99	1 (2%)	58,72,77	1.63	12 (20%)
26	0IE	5	303	-	42,45,45	1.43	6 (14%)	49,63,63	1.52	9 (18%)
25	CLA	4	315	10	49,53,73	1.49	8 (16%)	59,89,113	1.46	4 (6%)
25	CLA	c	607	-	69,73,73	1.25	11 (15%)	83,113,113	1.33	5 (6%)
25	CLA	p	314	-	59,63,73	1.34	10 (16%)	71,101,113	1.36	6 (8%)
25	CLA	a	610	-	45,49,73	1.52	8 (17%)	54,84,113	1.52	6 (11%)
25	CLA	A	603	19	69,73,73	1.26	11 (15%)	83,113,113	1.38	7 (8%)
26	0IE	7	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.54	9 (18%)
24	CHL	6	304	12	52,56,74	2.23	18 (34%)	58,92,114	3.18	25 (43%)
24	CHL	9	309	-	50,54,74	2.32	19 (38%)	56,90,114	3.23	25 (44%)
25	CLA	b	616	18	51,55,73	1.43	9 (17%)	61,91,113	1.48	5 (8%)
24	CHL	8	303	17	58,62,74	2.14	18 (31%)	65,99,114	3.04	27 (41%)
24	CHL	g	305	17	70,74,74	1.92	18 (25%)	80,114,114	2.78	27 (33%)
25	CLA	p	307	12	60,64,73	1.33	9 (15%)	72,102,113	1.39	5 (6%)
33	LMG	C	618	-	42,42,55	0.99	2 (4%)	50,50,63	1.23	4 (8%)
25	CLA	S	611	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
26	0IE	9	303	-	42,45,45	1.45	6 (14%)	49,63,63	1.74	11 (22%)
31	8CT	c	615	-	40,41,41	4.62	23 (57%)	50,56,56	2.73	17 (34%)
25	CLA	c	606	20	57,61,73	1.37	10 (17%)	68,98,113	1.41	6 (8%)
29	0UR	7	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.58	12 (20%)
37	DGD	c	619	-	56,56,67	0.95	3 (5%)	70,70,81	1.23	5 (7%)
25	CLA	q	313	-	67,71,73	1.25	8 (11%)	80,110,113	1.29	5 (6%)
23	HEM	E	201	2	50,50,50	1.35	6 (12%)	66,82,82	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	6	308	-	47,51,74	2.33	18 (38%)	52,86,114	3.35	24 (46%)
25	CLA	B	603	18	69,73,73	1.25	11 (15%)	83,113,113	1.31	7 (8%)
25	CLA	6	315	12	49,53,73	1.49	10 (20%)	59,89,113	1.47	6 (10%)
25	CLA	9	306	-	60,64,73	1.35	8 (13%)	72,102,113	1.34	5 (6%)
34	OEX	A	602	19	0,14,14	-	-	-		
25	CLA	S	616	-	49,53,73	1.47	9 (18%)	59,89,113	1.43	5 (8%)
25	CLA	2	314	-	59,63,73	1.33	10 (16%)	71,101,113	1.34	7 (9%)
24	CHL	q	309	-	57,61,74	2.10	18 (31%)	64,98,114	3.13	29 (45%)
25	CLA	p	316	-	49,53,73	1.47	10 (20%)	59,89,113	1.46	4 (6%)
24	CHL	g	310	-	51,55,74	2.29	19 (37%)	57,91,114	3.20	25 (43%)
24	CHL	R	605	-	46,50,74	2.26	19 (41%)	51,85,114	3.46	27 (52%)
25	CLA	n	315	17	49,53,73	1.48	10 (20%)	59,89,113	1.45	4 (6%)
24	CHL	g	318	17	46,50,74	2.32	18 (39%)	51,85,114	3.42	26 (50%)
25	CLA	g	307	-	57,61,73	1.39	8 (14%)	68,98,113	1.34	5 (7%)
30	LHG	c	617	-	31,31,48	1.31	5 (16%)	34,37,54	1.14	3 (8%)
25	CLA	2	307	11	47,51,73	1.48	9 (19%)	56,86,113	1.45	5 (8%)
34	OEX	a	602	19	0,14,14	-	-	-		
24	CHL	p	309	12	47,51,74	2.35	18 (38%)	52,86,114	3.38	25 (48%)
24	CHL	N	305	-	64,68,74	1.98	19 (29%)	72,106,114	2.88	28 (38%)
25	CLA	A	605	-	53,57,73	1.40	9 (16%)	62,93,113	1.45	7 (11%)
25	CLA	n	314	-	67,71,73	1.27	8 (11%)	80,110,113	1.30	5 (6%)
29	0UR	1	301	-	50,53,58	0.99	2 (4%)	58,72,77	1.96	17 (29%)
35	PHO	d	403	-	58,69,69	1.95	9 (15%)	56,99,99	1.54	8 (14%)
25	CLA	p	315	30	67,71,73	1.25	10 (14%)	80,110,113	1.39	6 (7%)
25	CLA	B	607	18	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
35	PHO	A	606	-	58,69,69	1.95	11 (18%)	56,99,99	1.49	7 (12%)
25	CLA	b	615	18	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
25	CLA	y	308	-	54,58,73	1.39	10 (18%)	65,95,113	1.44	9 (13%)
30	LHG	A	601	-	44,44,48	1.13	5 (11%)	47,50,54	0.98	2 (4%)
25	CLA	Y	314	30	67,71,73	1.26	9 (13%)	80,110,113	1.27	4 (5%)
25	CLA	G	308	-	54,58,73	1.40	7 (12%)	65,95,113	1.40	7 (10%)
24	CHL	n	309	-	50,54,74	2.18	19 (38%)	56,90,114	3.36	29 (51%)
25	CLA	2	317	-	53,57,73	1.40	9 (16%)	62,93,113	1.43	5 (8%)
25	CLA	B	614	18	60,64,73	1.32	9 (15%)	72,102,113	1.34	5 (6%)
26	0IE	2	303	-	42,45,45	1.42	6 (14%)	49,63,63	1.52	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	8CT	c	614	-	40,41,41	4.56	23 (57%)	50,56,56	2.70	21 (42%)
24	CHL	7	309	12	47,51,74	2.36	18 (38%)	52,86,114	3.38	25 (48%)
31	8CT	c	613	-	40,41,41	4.60	23 (57%)	50,56,56	2.70	21 (42%)
25	CLA	g	316	17	49,53,73	1.47	10 (20%)	59,89,113	1.48	4 (6%)
25	CLA	3	315	12	49,53,73	1.49	10 (20%)	59,89,113	1.46	6 (10%)
31	8CT	C	614	-	40,41,41	4.56	23 (57%)	50,56,56	2.68	21 (42%)
25	CLA	d	404	21	69,73,73	1.24	10 (14%)	83,113,113	1.33	7 (8%)
28	NEX	r	317	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
24	CHL	6	317	12	46,50,74	2.37	18 (39%)	51,85,114	3.43	28 (54%)
24	CHL	G	311	-	58,62,74	2.13	18 (31%)	65,99,114	3.08	27 (41%)
25	CLA	S	604	-	47,51,73	1.47	8 (17%)	56,86,113	1.46	5 (8%)
25	CLA	B	616	18	51,55,73	1.43	9 (17%)	61,91,113	1.49	5 (8%)
31	8CT	T	101	-	40,41,41	4.64	23 (57%)	50,56,56	3.04	18 (36%)
24	CHL	1	309	-	47,51,74	2.31	18 (38%)	52,86,114	3.28	24 (46%)
25	CLA	7	314	-	59,63,73	1.34	10 (16%)	71,101,113	1.36	6 (8%)
30	LHG	D	408	-	38,38,48	1.21	5 (13%)	41,44,54	1.06	2 (4%)
24	CHL	7	306	-	68,72,74	1.84	18 (26%)	77,111,114	2.93	32 (41%)
25	CLA	q	306	28	54,58,73	1.40	10 (18%)	65,95,113	1.40	8 (12%)
25	CLA	2	308	-	54,58,73	1.40	8 (14%)	65,95,113	1.45	7 (10%)
25	CLA	D	404	21	69,73,73	1.24	11 (15%)	83,113,113	1.32	8 (9%)
25	CLA	N	315	17	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
28	NEX	2	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
28	NEX	r	301	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
31	8CT	a	608	-	40,41,41	4.63	23 (57%)	50,56,56	2.66	20 (40%)
33	LMG	W	201	-	30,30,55	1.14	2 (6%)	38,38,63	1.37	6 (15%)
24	CHL	8	307	17	47,51,74	2.24	18 (38%)	52,86,114	3.34	26 (50%)
25	CLA	7	307	12	60,64,73	1.33	8 (13%)	72,102,113	1.40	5 (6%)
31	8CT	C	615	-	40,41,41	4.62	23 (57%)	50,56,56	2.75	18 (36%)
24	CHL	s	409	-	51,55,74	2.20	18 (35%)	57,91,114	3.21	25 (43%)
25	CLA	y	317	17	59,63,73	1.33	10 (16%)	70,100,113	1.40	7 (10%)
29	0UR	y	301	-	50,53,58	0.98	1 (2%)	58,72,77	1.63	14 (24%)
26	0IE	y	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.50	9 (18%)
25	CLA	R	603	-	51,55,73	1.42	7 (13%)	61,91,113	1.44	5 (8%)
29	0UR	G	301	-	50,53,58	0.95	1 (2%)	58,72,77	1.75	15 (25%)
25	CLA	c	603	20	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	d	405	21	69,73,73	1.24	9 (13%)	83,113,113	1.34	5 (6%)
29	0UR	n	301	-	50,53,58	0.95	1 (2%)	58,72,77	1.81	12 (20%)
25	CLA	q	315	17	47,51,73	1.48	10 (21%)	56,86,113	1.44	4 (7%)
24	CHL	3	317	12	46,50,74	2.37	19 (41%)	51,85,114	3.44	27 (52%)
25	CLA	S	612	-	59,63,73	1.35	10 (16%)	70,100,113	1.37	6 (8%)
25	CLA	8	313	17	49,53,73	1.47	9 (18%)	59,89,113	1.47	4 (6%)
25	CLA	4	313	-	59,63,73	1.36	8 (13%)	71,101,113	1.35	8 (11%)
24	CHL	u	305	12	70,74,74	1.97	18 (25%)	80,114,114	2.81	27 (33%)
24	CHL	p	306	-	68,72,74	1.84	18 (26%)	77,111,114	2.94	32 (41%)
29	0UR	4	301	-	50,53,58	0.99	2 (4%)	58,72,77	1.96	17 (29%)
24	CHL	5	309	11	47,51,74	2.31	17 (36%)	52,86,114	3.35	24 (46%)
31	8CT	b	617	-	40,41,41	4.66	23 (57%)	50,56,56	2.84	18 (36%)
25	CLA	b	601	-	49,53,73	1.46	10 (20%)	59,89,113	1.47	6 (10%)
24	CHL	Y	317	17	46,50,74	2.27	18 (39%)	51,85,114	3.43	27 (52%)
24	CHL	g	313	-	70,74,74	1.98	18 (25%)	80,114,114	2.76	29 (36%)
27	XAT	R	615	-	39,47,47	0.91	0	54,74,74	2.74	20 (37%)
25	CLA	C	610	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
33	LMG	D	401	-	48,48,55	0.91	2 (4%)	56,56,63	1.17	5 (8%)
24	CHL	y	313	-	70,74,74	1.89	19 (27%)	80,114,114	2.75	26 (32%)
24	CHL	G	312	-	55,59,74	2.18	19 (34%)	62,96,114	3.10	27 (43%)
25	CLA	q	305	17	58,62,73	1.36	9 (15%)	69,99,113	1.39	5 (7%)
24	CHL	4	312	-	50,54,74	2.29	18 (36%)	56,90,114	3.18	25 (44%)
24	CHL	N	312	-	60,64,74	2.06	18 (30%)	68,102,114	2.99	28 (41%)
25	CLA	8	306	-	54,58,73	1.40	9 (16%)	65,95,113	1.40	7 (10%)
24	CHL	R	602	-	51,55,74	2.16	19 (37%)	57,91,114	3.25	26 (45%)
24	CHL	Y	309	-	51,55,74	2.13	18 (35%)	57,91,114	3.31	28 (49%)
24	CHL	u	310	-	50,54,74	2.34	19 (38%)	56,90,114	3.23	25 (44%)
26	0IE	g	302	-	42,45,45	1.42	6 (14%)	49,63,63	1.58	10 (20%)
24	CHL	u	311	-	50,54,74	2.31	19 (38%)	56,90,114	3.23	24 (42%)
24	CHL	S	608	-	51,55,74	2.19	19 (37%)	57,91,114	3.23	27 (47%)
26	0IE	3	303	-	42,45,45	1.44	6 (14%)	49,63,63	1.70	9 (18%)
25	CLA	B	609	18	69,73,73	1.24	9 (13%)	83,113,113	1.32	8 (9%)
28	NEX	5	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	b	611	18	69,73,73	1.25	9 (13%)	83,113,113	1.39	7 (8%)
24	CHL	p	310	-	50,54,74	2.30	18 (36%)	56,90,114	3.23	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	c	601	20	69,73,73	1.24	10 (14%)	83,113,113	1.40	9 (10%)
24	CHL	u	313	-	47,51,74	2.32	17 (36%)	52,86,114	3.32	25 (48%)
24	CHL	y	309	17	47,51,74	2.23	17 (36%)	52,86,114	3.38	25 (48%)
39	PL9	d	406	-	55,55,55	1.68	12 (21%)	68,69,69	1.57	12 (17%)
24	CHL	5	313	-	46,50,74	2.33	18 (39%)	51,85,114	3.35	24 (47%)
31	8CT	s	416	-	40,41,41	4.74	25 (62%)	50,56,56	7.31	22 (44%)
33	LMG	i	101	-	48,48,55	0.92	2 (4%)	56,56,63	1.20	4 (7%)
25	CLA	9	315	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
25	CLA	C	603	20	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
28	NEX	7	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
24	CHL	n	310	-	57,61,74	2.17	19 (33%)	64,98,114	3.11	28 (43%)
25	CLA	b	602	18	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
25	CLA	r	314	-	51,55,73	1.46	7 (13%)	61,91,113	1.37	5 (8%)
24	CHL	Y	304	17	70,74,74	1.81	18 (25%)	80,114,114	2.88	29 (36%)
25	CLA	5	316	-	49,53,73	1.47	10 (20%)	59,89,113	1.47	4 (6%)
24	CHL	1	310	-	47,51,74	2.24	18 (38%)	52,86,114	3.31	25 (48%)
25	CLA	s	405	-	47,51,73	1.47	8 (17%)	56,86,113	1.46	6 (10%)
30	LHG	g	319	-	42,42,48	1.16	5 (11%)	45,48,54	0.99	2 (4%)
29	0UR	q	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.79	14 (24%)
32	SQD	d	409	-	43,44,54	1.06	5 (11%)	52,55,65	1.57	8 (15%)
25	CLA	9	314	30	67,71,73	1.27	7 (10%)	80,110,113	1.33	5 (6%)
24	CHL	8	304	17	64,68,74	1.96	19 (29%)	72,106,114	2.91	29 (40%)
37	DGD	C	620	-	56,56,67	0.95	2 (3%)	70,70,81	1.21	6 (8%)
30	LHG	a	601	-	44,44,48	1.12	5 (11%)	47,50,54	0.98	3 (6%)
24	CHL	y	306	-	68,72,74	1.85	18 (26%)	77,111,114	2.91	29 (37%)
25	CLA	B	613	18	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
25	CLA	u	307	-	60,64,73	1.35	7 (11%)	72,102,113	1.34	4 (5%)
24	CHL	n	311	-	54,58,74	2.13	20 (37%)	59,94,114	3.19	25 (42%)
24	CHL	r	307	-	52,56,74	2.19	17 (32%)	58,92,114	3.20	25 (43%)
26	0IE	8	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.52	10 (20%)
25	CLA	g	308	-	54,58,73	1.40	8 (14%)	65,95,113	1.40	7 (10%)
24	CHL	Y	308	17	47,51,74	2.24	17 (36%)	52,86,114	3.38	24 (46%)
24	CHL	n	304	17	58,62,74	2.16	18 (31%)	65,99,114	3.04	27 (41%)
25	CLA	S	603	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	6 (10%)
24	CHL	7	311	-	50,54,74	2.25	17 (34%)	56,90,114	3.22	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	G	310	-	51,55,74	2.28	19 (37%)	57,91,114	3.19	25 (43%)
24	CHL	s	407	-	50,54,74	2.25	19 (38%)	56,90,114	3.21	25 (44%)
25	CLA	B	601	-	49,53,73	1.46	10 (20%)	59,89,113	1.47	6 (10%)
26	0IE	Y	303	-	42,45,45	1.39	6 (14%)	49,63,63	1.50	8 (16%)
24	CHL	6	312	-	47,51,74	2.31	17 (36%)	52,86,114	3.28	24 (46%)
30	LHG	N	318	-	42,42,48	1.17	6 (14%)	45,48,54	0.97	2 (4%)
28	NEX	9	319	-	38,46,46	0.95	2 (5%)	50,70,70	4.90	19 (38%)
24	CHL	5	310	-	46,50,74	2.29	19 (41%)	51,85,114	3.39	24 (47%)
31	8CT	B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.88	18 (36%)
25	CLA	C	616	20	50,54,73	1.44	10 (20%)	60,90,113	1.49	7 (11%)
24	CHL	R	607	-	52,56,74	2.13	19 (36%)	58,92,114	3.32	27 (46%)
24	CHL	2	309	11	47,51,74	2.29	18 (38%)	52,86,114	3.34	24 (46%)
24	CHL	G	305	17	70,74,74	1.91	18 (25%)	80,114,114	2.79	27 (33%)
24	CHL	q	316	-	46,50,74	2.39	19 (41%)	51,85,114	3.42	25 (49%)
26	0IE	p	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.60	12 (24%)
24	CHL	1	304	-	46,50,74	2.40	18 (39%)	51,85,114	3.40	26 (50%)
25	CLA	2	315	-	67,71,73	1.26	8 (11%)	80,110,113	1.31	5 (6%)
25	CLA	c	609	20	69,73,73	1.27	9 (13%)	83,113,113	1.36	9 (10%)
24	CHL	s	414	-	46,50,74	2.29	18 (39%)	51,85,114	3.43	27 (52%)
24	CHL	1	312	10	50,54,74	2.29	18 (36%)	56,90,114	3.19	24 (42%)
25	CLA	B	611	18	69,73,73	1.25	9 (13%)	83,113,113	1.39	7 (8%)
24	CHL	4	305	-	50,54,74	2.23	19 (38%)	56,90,114	3.29	26 (46%)
28	NEX	1	303	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
30	LHG	Y	318	25	42,42,48	1.16	5 (11%)	45,48,54	1.10	3 (6%)
24	CHL	3	308	-	47,51,74	2.33	18 (38%)	52,86,114	3.34	24 (46%)
24	CHL	7	310	-	50,54,74	2.31	19 (38%)	56,90,114	3.24	26 (46%)
25	CLA	8	305	17	58,62,73	1.35	9 (15%)	69,99,113	1.38	5 (7%)
25	CLA	b	608	-	59,63,73	1.35	9 (15%)	71,101,113	1.37	7 (9%)
30	LHG	p	319	25	42,42,48	1.17	5 (11%)	45,48,54	1.02	3 (6%)
25	CLA	u	308	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
25	CLA	N	307	-	54,58,73	1.40	9 (16%)	65,95,113	1.41	7 (10%)
25	CLA	a	603	19	69,73,73	1.26	11 (15%)	83,113,113	1.38	7 (8%)
25	CLA	s	404	-	49,53,73	1.47	8 (16%)	59,89,113	1.45	6 (10%)
32	SQD	A	609	-	44,45,54	1.06	5 (11%)	53,56,65	1.55	10 (18%)
35	PHO	D	403	-	58,69,69	1.94	9 (15%)	56,99,99	1.53	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	r	302	8	50,54,74	2.32	18 (36%)	56,90,114	3.24	25 (44%)
24	CHL	p	318	12	46,50,74	2.33	18 (39%)	51,85,114	3.39	27 (52%)
25	CLA	1	315	10	49,53,73	1.50	8 (16%)	59,89,113	1.46	4 (6%)
29	0UR	8	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.78	14 (24%)
24	CHL	3	304	12	52,56,74	2.21	19 (36%)	58,92,114	3.17	24 (41%)
24	CHL	5	311	-	51,55,74	2.27	19 (37%)	57,91,114	3.13	25 (43%)
24	CHL	R	601	8	50,54,74	2.33	18 (36%)	56,90,114	3.26	25 (44%)
25	CLA	b	613	18	69,73,73	1.26	10 (14%)	83,113,113	1.28	7 (8%)
24	CHL	g	309	-	47,51,74	2.36	18 (38%)	52,86,114	3.36	24 (46%)
31	8CT	x	601	-	40,41,41	4.63	23 (57%)	50,56,56	2.59	19 (38%)
25	CLA	r	310	8	59,63,73	1.34	10 (16%)	71,101,113	1.36	5 (7%)
25	CLA	c	602	20	69,73,73	1.26	11 (15%)	83,113,113	1.33	6 (7%)
25	CLA	g	315	-	64,68,73	1.30	8 (12%)	77,107,113	1.29	5 (6%)
30	LHG	4	318	-	41,41,48	1.19	6 (14%)	44,47,54	0.97	3 (6%)
24	CHL	Y	310	-	58,62,74	2.03	19 (32%)	65,99,114	3.19	29 (44%)
28	NEX	y	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
33	LMG	B	619	-	41,41,55	0.97	2 (4%)	49,49,63	1.30	4 (8%)
24	CHL	s	406	-	50,54,74	2.24	18 (36%)	56,90,114	3.23	23 (41%)
25	CLA	B	605	18	69,73,73	1.25	10 (14%)	83,113,113	1.27	7 (8%)
28	NEX	3	318	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
28	NEX	G	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
24	CHL	5	318	11	46,50,74	2.38	18 (39%)	51,85,114	3.41	25 (49%)
24	CHL	n	305	-	64,68,74	1.98	19 (29%)	72,106,114	2.88	28 (38%)
26	0IE	u	303	-	42,45,45	1.45	6 (14%)	49,63,63	1.67	10 (20%)
29	0UR	p	301	-	50,53,58	0.93	1 (2%)	58,72,77	1.59	12 (20%)
25	CLA	Y	307	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	9 (13%)
25	CLA	S	609	-	59,63,73	1.32	10 (16%)	71,101,113	1.34	5 (7%)
24	CHL	S	606	-	50,54,74	2.25	19 (38%)	56,90,114	3.22	25 (44%)
24	CHL	6	305	-	52,56,74	2.20	19 (36%)	58,92,114	3.16	26 (44%)
25	CLA	N	306	17	58,62,73	1.36	8 (13%)	69,99,113	1.38	6 (8%)
28	NEX	S	617	-	38,46,46	0.95	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	a	605	-	53,57,73	1.39	9 (16%)	62,93,113	1.45	7 (11%)
24	CHL	9	304	12	70,74,74	1.93	18 (25%)	80,114,114	2.79	27 (33%)
24	CHL	4	311	-	48,52,74	2.21	18 (37%)	53,87,114	3.28	24 (45%)
25	CLA	s	411	-	48,52,73	1.51	11 (22%)	56,87,113	1.46	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	0IE	r	315	-	42,45,45	1.44	6 (14%)	49,63,63	1.54	10 (20%)
35	PHO	a	606	-	58,69,69	1.95	10 (17%)	56,99,99	1.49	7 (12%)
25	CLA	b	606	18	69,73,73	1.23	10 (14%)	83,113,113	1.36	7 (8%)
25	CLA	b	603	18	69,73,73	1.25	11 (15%)	83,113,113	1.31	8 (9%)
25	CLA	c	610	-	69,73,73	1.24	11 (15%)	83,113,113	1.32	9 (10%)
32	SQD	B	618	-	53,54,54	0.95	5 (9%)	62,65,65	1.55	11 (17%)
25	CLA	4	307	28	45,49,73	1.52	9 (20%)	54,84,113	1.50	7 (12%)
25	CLA	u	317	12	59,63,73	1.37	9 (15%)	70,100,113	1.35	5 (7%)
24	CHL	3	310	-	50,54,74	2.33	18 (36%)	56,90,114	3.20	25 (44%)
24	CHL	p	312	-	51,55,74	2.11	18 (35%)	57,91,114	3.32	28 (49%)
24	CHL	7	318	12	46,50,74	2.34	18 (39%)	51,85,114	3.39	27 (52%)
39	PL9	D	406	-	55,55,55	1.67	12 (21%)	68,69,69	1.57	12 (17%)
28	NEX	6	303	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
30	LHG	1	318	-	41,41,48	1.19	6 (14%)	44,47,54	0.97	3 (6%)
33	LMG	m	101	-	41,41,55	0.98	2 (4%)	49,49,63	1.23	4 (8%)
24	CHL	9	305	-	68,72,74	1.94	19 (27%)	77,111,114	2.82	27 (35%)
30	LHG	d	408	-	38,38,48	0.98	2 (5%)	41,44,54	1.24	4 (9%)
24	CHL	9	310	-	50,54,74	2.32	19 (38%)	56,90,114	3.22	24 (42%)
25	CLA	B	604	18	66,70,73	1.28	9 (13%)	79,109,113	1.41	8 (10%)
25	CLA	6	316	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	6 (10%)
31	8CT	X	601	-	40,41,41	4.63	23 (57%)	50,56,56	2.58	19 (38%)
25	CLA	r	304	-	51,55,73	1.42	8 (15%)	61,91,113	1.46	5 (8%)
24	CHL	3	312	-	47,51,74	2.32	17 (36%)	52,86,114	3.28	25 (48%)
25	CLA	6	307	-	47,51,73	1.48	8 (17%)	56,86,113	1.46	4 (7%)
25	CLA	Y	316	17	59,63,73	1.33	10 (16%)	70,100,113	1.41	6 (8%)
24	CHL	8	308	-	50,54,74	2.21	18 (36%)	56,90,114	3.31	27 (48%)
25	CLA	1	306	-	48,52,73	1.47	8 (16%)	56,87,113	1.45	6 (10%)
25	CLA	q	312	-	59,63,73	1.33	10 (16%)	71,101,113	1.39	7 (9%)
32	SQD	a	609	-	44,45,54	1.05	5 (11%)	53,56,65	1.67	10 (18%)
31	8CT	D	410	-	40,41,41	4.70	23 (57%)	50,56,56	2.47	18 (36%)
24	CHL	p	313	-	47,51,74	2.22	18 (38%)	52,86,114	3.29	23 (44%)
28	NEX	n	303	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	18 (36%)
25	CLA	G	315	-	64,68,73	1.30	8 (12%)	77,107,113	1.29	5 (6%)
25	CLA	Y	313	17	59,63,73	1.34	10 (16%)	71,101,113	1.37	8 (11%)
33	LMG	d	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.14	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	N	313	-	59,63,73	1.34	8 (13%)	71,101,113	1.37	8 (11%)
25	CLA	8	314	-	47,51,73	1.48	10 (21%)	56,86,113	1.46	5 (8%)
25	CLA	6	314	-	45,49,73	1.51	7 (15%)	54,84,113	1.50	6 (11%)
28	NEX	4	303	25	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
30	LHG	2	319	-	39,39,48	1.20	5 (12%)	42,45,54	1.06	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	G	313	-	-	23/41/117/117	-
25	CLA	1	307	-	-	4/10/86/115	-
25	CLA	G	314	-	-	4/27/103/115	-
25	CLA	y	316	17	-	6/15/91/115	-
24	CHL	2	310	-	-	2/12/88/117	-
25	CLA	7	316	12	-	4/15/91/115	-
26	0IE	G	303	-	-	0/33/72/72	0/2/2/2
24	CHL	4	310	-	-	2/14/90/117	-
29	0UR	u	301	-	-	10/42/81/86	0/2/2/2
24	CHL	q	308	-	-	6/17/93/117	-
30	LHG	d	407	-	-	27/53/53/53	-
31	8CT	S	614	-	-	6/29/63/63	0/2/2/2
25	CLA	R	609	8	-	3/27/103/115	-
24	CHL	R	606	-	-	8/20/96/117	-
26	0IE	R	614	-	-	1/33/72/72	0/2/2/2
30	LHG	G	319	-	-	23/47/47/53	-
25	CLA	C	609	20	-	6/39/115/115	-
30	LHG	9	318	25	-	25/47/47/53	-
24	CHL	q	304	17	-	17/34/110/117	-
25	CLA	4	314	-	-	6/10/86/115	-
30	LHG	5	319	-	-	20/47/47/53	-
25	CLA	3	316	-	-	8/15/91/115	-
25	CLA	7	308	-	-	6/21/97/115	-
37	DGD	C	619	-	-	27/39/79/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	s	413	-	-	9/27/103/115	-
31	8CT	d	410	-	-	9/29/63/63	0/2/2/2
24	CHL	2	305	11	-	6/15/91/117	-
25	CLA	Y	306	17	-	5/25/101/115	-
25	CLA	3	307	-	-	6/13/89/115	-
25	CLA	4	306	-	-	6/13/90/115	-
25	CLA	6	313	-	-	2/10/86/115	-
24	CHL	s	408	-	-	6/17/93/117	-
25	CLA	C	608	20	-	10/35/111/115	-
24	CHL	1	308	10	-	2/14/90/117	-
24	CHL	G	309	-	-	2/14/90/117	-
25	CLA	g	317	17	-	6/27/103/115	-
25	CLA	u	314	-	-	3/27/103/115	-
25	CLA	r	305	-	-	3/10/86/115	-
25	CLA	y	314	17	-	5/27/103/115	-
30	LHG	A	612	-	-	15/48/48/53	-
24	CHL	2	318	11	-	6/12/88/117	-
30	LHG	C	617	-	-	17/36/36/53	-
25	CLA	9	316	12	-	11/27/103/115	-
24	CHL	g	306	-	-	26/39/115/117	-
24	CHL	u	318	-	-	6/12/88/117	-
24	CHL	Y	312	-	-	19/41/117/117	-
24	CHL	1	311	-	-	3/15/91/117	-
24	CHL	y	310	-	-	5/19/95/117	-
25	CLA	C	602	20	-	20/39/115/115	-
24	CHL	5	305	11	-	7/15/91/117	-
25	CLA	B	606	18	-	18/39/115/115	-
25	CLA	A	604	-	-	9/39/115/115	-
28	NEX	N	303	-	-	4/27/83/83	0/3/3/3
25	CLA	B	610	-	-	4/39/115/115	-
25	CLA	n	306	17	-	9/26/102/115	-
24	CHL	S	607	-	-	5/17/93/117	-
32	SQD	D	409	-	-	13/39/59/69	0/1/1/1
24	CHL	q	303	17	-	8/27/103/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	6	306	-	-	5/10/86/115	-
24	CHL	r	309	-	-	6/17/93/117	-
25	CLA	s	410	-	-	5/27/103/115	-
25	CLA	R	613	-	-	9/18/94/115	-
31	8CT	s	415	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	-	-	12/27/103/115	-
31	8CT	V	401	-	-	11/29/63/63	0/2/2/2
25	CLA	R	612	-	-	7/15/91/115	-
24	CHL	u	309	12	-	2/14/90/117	-
28	NEX	p	304	-	-	5/27/83/83	0/3/3/3
29	0UR	g	301	-	-	10/42/81/86	0/2/2/2
25	CLA	3	313	-	-	2/10/86/115	-
24	CHL	S	605	-	-	6/17/93/117	-
23	HEM	f	201	2,9	-	1/14/54/54	-
25	CLA	2	316	-	-	4/15/91/115	-
24	CHL	p	305	12	-	17/41/117/117	-
24	CHL	q	311	-	-	11/29/105/117	-
25	CLA	A	610	-	-	4/10/86/115	-
24	CHL	u	306	-	-	17/39/115/117	-
24	CHL	1	317	-	-	7/12/88/117	-
30	LHG	n	318	-	-	20/47/47/53	-
24	CHL	2	313	-	-	4/12/88/117	-
25	CLA	D	405	21	-	12/39/115/115	-
24	CHL	y	311	-	-	12/27/103/117	-
24	CHL	N	304	17	-	8/27/103/117	-
24	CHL	S	613	-	-	3/12/88/117	-
30	LHG	7	319	25	-	24/41/41/53	-
26	0IE	7	302	-	-	4/33/72/72	0/2/2/2
24	CHL	9	311	-	-	7/19/95/117	-
25	CLA	9	307	-	-	9/21/97/115	-
25	CLA	A	607	19	-	4/33/109/115	-
26	0IE	g	303	-	-	0/33/72/72	0/2/2/2
25	CLA	y	307	17	-	5/25/101/115	-
25	CLA	C	605	20	-	9/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	g	304	-	-	5/27/83/83	0/3/3/3
25	CLA	R	611	8	-	8/15/91/115	-
24	CHL	N	309	-	-	7/17/93/117	-
24	CHL	S	601	13	-	12/17/93/117	-
24	CHL	n	308	17	-	4/14/90/117	-
31	8CT	v	401	-	-	11/29/63/63	0/2/2/2
25	CLA	3	306	-	-	5/10/86/115	-
25	CLA	b	604	18	-	16/36/112/115	-
25	CLA	C	611	20	-	13/39/115/115	-
26	0IE	5	302	-	-	2/33/72/72	0/2/2/2
24	CHL	7	312	-	-	7/19/95/117	-
25	CLA	n	307	-	-	5/21/97/115	-
24	CHL	4	308	10	-	2/14/90/117	-
25	CLA	9	313	-	-	3/27/103/115	-
25	CLA	C	607	-	-	11/39/115/115	-
24	CHL	n	312	-	-	12/29/105/117	-
25	CLA	r	311	-	-	6/15/91/115	-
26	0IE	1	302	-	-	2/33/72/72	0/2/2/2
25	CLA	B	602	18	-	13/39/115/115	-
33	LMG	w	201	-	-	17/31/51/70	0/1/1/1
24	CHL	9	317	-	-	6/12/88/117	-
26	0IE	6	302	-	-	4/33/69/72	0/2/2/2
37	DGD	c	618	-	-	27/39/79/95	0/2/2/2
25	CLA	7	315	30	-	15/37/113/115	-
25	CLA	N	314	-	-	7/37/113/115	-
25	CLA	C	604	-	-	17/39/115/115	-
24	CHL	y	312	-	-	5/23/99/117	-
30	LHG	y	319	25	-	25/47/47/53	-
30	LHG	D	407	-	-	29/53/53/53	-
25	CLA	g	314	-	-	4/27/103/115	-
25	CLA	b	614	18	-	13/29/105/115	-
24	CHL	N	310	-	-	9/26/102/117	-
25	CLA	5	307	11	-	7/13/89/115	-
24	CHL	2	306	-	-	10/19/95/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	p	311	-	-	3/17/93/117	-
25	CLA	c	608	20	-	10/35/111/115	-
24	CHL	9	308	12	-	2/14/90/117	-
25	CLA	u	315	-	-	13/37/113/115	-
29	0UR	9	301	-	-	10/42/81/86	0/2/2/2
26	0IE	y	302	-	-	2/33/72/72	0/2/2/2
24	CHL	3	311	-	-	5/15/91/117	-
24	CHL	r	303	-	-	6/19/95/117	-
24	CHL	4	317	-	-	8/12/88/117	-
25	CLA	y	315	30	-	12/37/113/115	-
25	CLA	G	307	-	-	6/25/101/115	-
25	CLA	8	311	-	-	3/27/103/115	-
24	CHL	y	305	17	-	11/41/117/117	-
24	CHL	7	305	12	-	17/41/117/117	-
25	CLA	G	317	-	-	6/27/103/115	-
24	CHL	r	308	-	-	11/20/96/117	-
25	CLA	b	605	18	-	16/39/115/115	-
29	0UR	6	301	-	-	9/42/81/86	0/2/2/2
25	CLA	r	312	8	-	8/15/91/115	-
26	0IE	3	302	-	-	4/33/69/72	0/2/2/2
25	CLA	C	612	20	-	10/26/102/115	-
24	CHL	g	311	-	-	8/27/103/117	-
28	NEX	s	401	25	-	4/27/83/83	0/3/3/3
24	CHL	N	311	-	-	7/22/98/117	-
25	CLA	1	316	10	-	1/12/88/115	-
28	NEX	u	304	-	-	5/27/83/83	0/3/3/3
26	0IE	G	302	-	-	2/33/72/72	0/2/2/2
25	CLA	5	315	-	-	10/37/113/115	-
24	CHL	Y	305	-	-	22/39/115/117	-
26	0IE	u	302	-	-	4/33/72/72	0/2/2/2
24	CHL	n	317	-	-	4/12/88/117	-
32	SQD	b	618	-	-	15/49/69/69	0/1/1/1
24	CHL	8	309	-	-	5/22/98/117	-
25	CLA	s	412	13	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	610	-	-	5/39/115/115	-
25	CLA	b	609	18	-	19/39/115/115	-
26	0IE	n	302	-	-	2/33/72/72	0/2/2/2
24	CHL	8	315	-	-	0/12/88/117	-
25	CLA	c	604	-	-	18/39/115/115	-
25	CLA	a	607	19	-	4/33/109/115	-
30	LHG	a	612	-	-	15/48/48/53	-
24	CHL	6	311	-	-	4/15/91/117	-
25	CLA	5	314	-	-	5/27/103/115	-
26	0IE	4	302	-	-	2/33/72/72	0/2/2/2
25	CLA	b	612	18	-	11/39/115/115	-
29	0UR	2	301	-	-	14/42/81/86	0/2/2/2
24	CHL	S	602	13	-	16/32/108/117	-
24	CHL	N	308	17	-	4/14/90/117	-
24	CHL	G	318	17	-	8/12/88/117	-
25	CLA	u	316	-	-	6/15/91/115	-
25	CLA	a	604	-	-	10/39/115/115	-
25	CLA	1	314	-	-	6/10/86/115	-
25	CLA	N	316	-	-	2/13/89/115	-
26	0IE	9	302	-	-	4/33/72/72	0/2/2/2
25	CLA	Y	315	17	-	6/15/91/115	-
29	0UR	3	301	-	-	9/42/81/86	0/2/2/2
24	CHL	3	305	-	-	10/20/96/117	-
25	CLA	r	313	-	-	7/15/91/115	-
25	CLA	c	611	20	-	13/39/115/115	-
24	CHL	Y	311	-	-	5/23/99/117	-
28	NEX	R	616	-	-	5/27/83/83	0/3/3/3
25	CLA	S	610	-	-	2/15/91/115	-
25	CLA	1	313	-	-	5/27/103/115	-
24	CHL	9	312	-	-	4/14/90/117	-
25	CLA	5	308	-	-	4/21/97/115	-
25	CLA	c	612	20	-	10/26/102/115	-
31	8CT	A	608	-	-	8/29/63/63	0/2/2/2
24	CHL	1	305	10	-	8/17/93/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	606	20	-	9/25/101/115	-
24	CHL	G	306	17	-	26/39/115/117	-
25	CLA	q	314	17	-	4/15/91/115	-
25	CLA	G	316	17	-	6/15/91/115	-
24	CHL	6	309	-	-	7/23/99/117	-
24	CHL	s	402	13	-	12/17/93/117	-
24	CHL	2	312	-	-	7/17/93/117	-
33	LMG	d	401	-	-	12/43/63/70	0/1/1/1
25	CLA	B	612	18	-	12/39/115/115	-
24	CHL	4	309	-	-	4/14/90/117	-
24	CHL	R	608	-	-	6/17/93/117	-
24	CHL	6	310	-	-	7/17/93/117	-
25	CLA	R	604	-	-	5/10/86/115	-
25	CLA	n	316	-	-	3/13/89/115	-
26	0IE	N	302	-	-	2/33/72/72	0/2/2/2
25	CLA	c	605	20	-	9/29/105/115	-
24	CHL	N	317	-	-	4/12/88/117	-
25	CLA	4	316	-	-	0/12/88/115	-
24	CHL	5	306	-	-	9/19/95/117	-
25	CLA	s	417	-	-	8/15/91/115	-
27	XAT	r	316	-	-	0/31/93/93	0/4/4/4
26	0IE	2	302	-	-	2/33/72/72	0/2/2/2
24	CHL	5	312	-	-	7/17/93/117	-
33	LMG	D	411	-	-	26/41/61/70	0/1/1/1
24	CHL	y	318	17	-	6/12/88/117	-
25	CLA	8	312	-	-	10/37/113/115	-
26	0IE	p	303	-	-	2/33/72/72	0/2/2/2
24	CHL	2	311	-	-	7/19/95/117	-
26	0IE	Y	302	-	-	2/33/72/72	0/2/2/2
24	CHL	g	312	-	-	5/23/99/117	-
24	CHL	q	307	17	-	2/14/90/117	-
26	0IE	q	302	-	-	2/33/72/72	0/2/2/2
25	CLA	B	615	18	-	4/39/115/115	-
25	CLA	R	610	-	-	4/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	5	317	11	-	9/20/96/115	-
25	CLA	3	314	-	-	4/10/86/115	-
31	8CT	t	101	-	-	12/29/63/63	0/2/2/2
24	CHL	7	313	-	-	5/14/90/117	-
25	CLA	b	607	18	-	14/39/115/115	-
29	0UR	N	301	-	-	10/42/81/86	0/2/2/2
31	8CT	C	613	-	-	8/29/63/63	0/2/2/2
25	CLA	p	308	-	-	7/21/97/115	-
31	8CT	S	615	-	-	12/29/63/63	0/2/2/2
24	CHL	4	304	-	-	2/12/88/117	-
24	CHL	q	310	-	-	5/22/98/117	-
24	CHL	s	403	13	-	17/32/108/117	-
25	CLA	p	317	12	-	9/27/103/115	-
25	CLA	n	313	-	-	6/27/103/115	-
24	CHL	3	309	-	-	7/23/99/117	-
25	CLA	7	317	12	-	9/24/100/115	-
25	CLA	C	601	20	-	14/39/115/115	-
24	CHL	r	306	-	-	6/12/88/117	-
24	CHL	u	312	-	-	7/19/95/117	-
24	CHL	8	310	-	-	11/29/105/117	-
24	CHL	Y	319	-	-	8/26/102/117	-
25	CLA	c	616	20	-	4/17/93/115	-
29	0UR	5	301	-	-	14/42/81/86	0/2/2/2
29	0UR	Y	301	-	-	12/42/81/86	0/2/2/2
26	0IE	5	303	-	-	0/33/72/72	0/2/2/2
25	CLA	4	315	10	-	8/15/91/115	-
25	CLA	c	607	-	-	11/39/115/115	-
25	CLA	p	314	-	-	5/27/103/115	-
25	CLA	a	610	-	-	4/10/86/115	-
25	CLA	A	603	19	-	13/39/115/115	-
26	0IE	7	303	-	-	2/33/72/72	0/2/2/2
24	CHL	6	304	12	-	8/20/96/117	-
24	CHL	9	309	-	-	9/17/93/117	-
25	CLA	b	616	18	-	6/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	8	303	17	-	8/27/103/117	-
24	CHL	g	305	17	-	21/41/117/117	-
25	CLA	p	307	12	-	8/29/105/115	-
33	LMG	C	618	-	-	17/37/57/70	0/1/1/1
25	CLA	S	611	13	-	6/15/91/115	-
26	0IE	9	303	-	-	5/33/72/72	0/2/2/2
31	8CT	c	615	-	-	12/29/63/63	0/2/2/2
25	CLA	c	606	20	-	9/25/101/115	-
29	0UR	7	301	-	-	8/42/81/86	0/2/2/2
37	DGD	c	619	-	-	17/44/84/95	0/2/2/2
25	CLA	q	313	-	-	8/37/113/115	-
23	HEM	E	201	2	-	0/14/54/54	-
24	CHL	6	308	-	-	2/14/90/117	-
25	CLA	B	603	18	-	12/39/115/115	-
25	CLA	6	315	12	-	7/15/91/115	-
25	CLA	9	306	-	-	6/29/105/115	-
25	CLA	S	616	-	-	8/15/91/115	-
25	CLA	2	314	-	-	5/27/103/115	-
24	CHL	q	309	-	-	10/26/102/117	-
25	CLA	p	316	-	-	4/15/91/115	-
24	CHL	g	310	-	-	7/19/95/117	-
24	CHL	R	605	-	-	4/12/88/117	-
25	CLA	n	315	17	-	6/15/91/115	-
24	CHL	g	318	17	-	8/12/88/117	-
25	CLA	g	307	-	-	6/25/101/115	-
30	LHG	c	617	-	-	17/36/36/53	-
25	CLA	2	307	11	-	6/13/89/115	-
24	CHL	p	309	12	-	1/14/90/117	-
24	CHL	N	305	-	-	16/34/110/117	-
25	CLA	A	605	-	-	7/20/96/115	-
25	CLA	n	314	-	-	6/37/113/115	-
29	0UR	1	301	-	-	13/42/81/86	0/2/2/2
35	PHO	d	403	-	-	10/37/103/103	0/5/6/6
25	CLA	p	315	30	-	15/37/113/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	607	18	-	15/39/115/115	-
35	PHO	A	606	-	-	9/37/103/103	0/5/6/6
25	CLA	b	615	18	-	5/39/115/115	-
25	CLA	y	308	-	-	9/21/97/115	-
30	LHG	A	601	-	-	24/49/49/53	-
25	CLA	Y	314	30	-	13/37/113/115	-
25	CLA	G	308	-	-	10/21/97/115	-
24	CHL	n	309	-	-	7/17/93/117	-
25	CLA	2	317	-	-	9/20/96/115	-
25	CLA	B	614	18	-	13/29/105/115	-
26	0IE	2	303	-	-	0/33/72/72	0/2/2/2
31	8CT	c	614	-	-	14/29/63/63	0/2/2/2
24	CHL	7	309	12	-	0/14/90/117	-
31	8CT	c	613	-	-	8/29/63/63	0/2/2/2
25	CLA	g	316	17	-	5/15/91/115	-
25	CLA	3	315	12	-	6/15/91/115	-
31	8CT	C	614	-	-	14/29/63/63	0/2/2/2
25	CLA	d	404	21	-	11/39/115/115	-
28	NEX	r	317	-	-	5/27/83/83	0/3/3/3
24	CHL	6	317	12	-	0/12/88/117	-
24	CHL	G	311	-	-	10/27/103/117	-
25	CLA	S	604	-	-	4/13/89/115	-
25	CLA	B	616	18	-	6/18/94/115	-
31	8CT	T	101	-	-	12/29/63/63	0/2/2/2
24	CHL	1	309	-	-	3/14/90/117	-
25	CLA	7	314	-	-	7/27/103/115	-
30	LHG	D	408	-	-	21/43/43/53	-
24	CHL	7	306	-	-	27/39/115/117	-
25	CLA	q	306	28	-	5/21/97/115	-
25	CLA	2	308	-	-	4/21/97/115	-
25	CLA	D	404	21	-	9/39/115/115	-
25	CLA	N	315	17	-	7/15/91/115	-
28	NEX	2	304	-	-	5/27/83/83	0/3/3/3
28	NEX	r	301	-	-	4/27/83/83	0/3/3/3
31	8CT	a	608	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	W	201	-	-	11/25/45/70	0/1/1/1
24	CHL	8	307	17	-	2/14/90/117	-
25	CLA	7	307	12	-	7/29/105/115	-
31	8CT	C	615	-	-	13/29/63/63	0/2/2/2
24	CHL	s	409	-	-	7/19/95/117	-
25	CLA	y	317	17	-	11/27/103/115	-
29	0UR	y	301	-	-	12/42/81/86	0/2/2/2
26	0IE	y	303	-	-	0/33/72/72	0/2/2/2
25	CLA	R	603	-	-	6/18/94/115	-
29	0UR	G	301	-	-	10/42/81/86	0/2/2/2
25	CLA	c	603	20	-	13/39/115/115	-
25	CLA	d	405	21	-	12/39/115/115	-
29	0UR	n	301	-	-	9/42/81/86	0/2/2/2
25	CLA	q	315	17	-	5/13/89/115	-
24	CHL	3	317	12	-	2/12/88/117	-
25	CLA	S	612	-	-	9/27/103/115	-
25	CLA	8	313	17	-	4/15/91/115	-
25	CLA	4	313	-	-	6/27/103/115	-
24	CHL	u	305	12	-	15/41/117/117	-
24	CHL	p	306	-	-	26/39/115/117	-
29	0UR	4	301	-	-	13/42/81/86	0/2/2/2
24	CHL	5	309	11	-	3/14/90/117	-
31	8CT	b	617	-	-	14/29/63/63	0/2/2/2
25	CLA	b	601	-	-	11/15/91/115	-
24	CHL	Y	317	17	-	6/12/88/117	-
24	CHL	g	313	-	-	21/41/117/117	-
27	XAT	R	615	-	-	0/31/93/93	0/4/4/4
25	CLA	C	610	-	-	10/39/115/115	-
33	LMG	D	401	-	-	10/43/63/70	0/1/1/1
24	CHL	y	313	-	-	19/41/117/117	-
24	CHL	G	312	-	-	5/23/99/117	-
25	CLA	q	305	17	-	10/26/102/115	-
24	CHL	4	312	-	-	6/17/93/117	-
24	CHL	N	312	-	-	11/29/105/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	8	306	-	-	6/21/97/115	-
24	CHL	R	602	-	-	5/19/95/117	-
24	CHL	Y	309	-	-	5/19/95/117	-
24	CHL	u	310	-	-	9/17/93/117	-
26	0IE	g	302	-	-	2/33/72/72	0/2/2/2
24	CHL	u	311	-	-	4/17/93/117	-
24	CHL	S	608	-	-	7/19/95/117	-
26	0IE	3	303	-	-	1/33/72/72	0/2/2/2
25	CLA	B	609	18	-	16/39/115/115	-
28	NEX	5	304	-	-	5/27/83/83	0/3/3/3
25	CLA	b	611	18	-	6/39/115/115	-
24	CHL	p	310	-	-	7/17/93/117	-
25	CLA	c	601	20	-	14/39/115/115	-
24	CHL	u	313	-	-	5/14/90/117	-
24	CHL	y	309	17	-	5/14/90/117	-
39	PL9	d	406	-	-	11/53/73/73	0/1/1/1
24	CHL	5	313	-	-	3/12/88/117	-
31	8CT	s	416	-	-	12/29/63/63	0/2/2/2
33	LMG	i	101	-	-	14/43/63/70	0/1/1/1
25	CLA	9	315	-	-	6/15/91/115	-
25	CLA	C	603	20	-	14/39/115/115	-
28	NEX	7	304	-	-	5/27/83/83	0/3/3/3
24	CHL	n	310	-	-	9/26/102/117	-
25	CLA	b	602	18	-	13/39/115/115	-
25	CLA	r	314	-	-	9/18/94/115	-
24	CHL	Y	304	17	-	15/41/117/117	-
25	CLA	5	316	-	-	4/15/91/115	-
24	CHL	1	310	-	-	2/14/90/117	-
25	CLA	s	405	-	-	4/13/89/115	-
30	LHG	g	319	-	-	23/47/47/53	-
29	0UR	q	301	-	-	10/42/81/86	0/2/2/2
32	SQD	d	409	-	-	13/39/59/69	0/1/1/1
25	CLA	9	314	30	-	14/37/113/115	-
24	CHL	8	304	17	-	15/34/110/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	620	-	-	25/44/84/95	0/2/2/2
30	LHG	a	601	-	-	25/49/49/53	-
24	CHL	y	306	-	-	22/39/115/117	-
25	CLA	B	613	18	-	10/39/115/115	-
25	CLA	u	307	-	-	6/29/105/115	-
24	CHL	n	311	-	-	7/22/98/117	-
24	CHL	r	307	-	-	7/20/96/117	-
26	0IE	8	302	-	-	2/33/72/72	0/2/2/2
25	CLA	g	308	-	-	8/21/97/115	-
24	CHL	Y	308	17	-	5/14/90/117	-
24	CHL	n	304	17	-	8/27/103/117	-
25	CLA	S	603	-	-	5/15/91/115	-
24	CHL	7	311	-	-	2/17/93/117	-
24	CHL	G	310	-	-	9/19/95/117	-
24	CHL	s	407	-	-	6/17/93/117	-
25	CLA	B	601	-	-	11/15/91/115	-
26	0IE	Y	303	-	-	0/33/72/72	0/2/2/2
24	CHL	6	312	-	-	3/14/90/117	-
30	LHG	N	318	-	-	18/47/47/53	-
28	NEX	9	319	-	-	5/27/83/83	0/3/3/3
24	CHL	5	310	-	-	4/12/88/117	-
31	8CT	B	617	-	-	13/29/63/63	0/2/2/2
25	CLA	C	616	20	-	4/17/93/115	-
24	CHL	R	607	-	-	11/20/96/117	-
24	CHL	2	309	11	-	3/14/90/117	-
24	CHL	G	305	17	-	21/41/117/117	-
24	CHL	q	316	-	-	1/12/88/117	-
26	0IE	p	302	-	-	4/33/72/72	0/2/2/2
24	CHL	1	304	-	-	2/12/88/117	-
25	CLA	2	315	-	-	10/37/113/115	-
25	CLA	c	609	20	-	6/39/115/115	-
24	CHL	s	414	-	-	3/12/88/117	-
24	CHL	1	312	10	-	6/17/93/117	-
25	CLA	B	611	18	-	6/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	4	305	-	-	8/17/93/117	-
28	NEX	1	303	-	-	5/27/83/83	0/3/3/3
30	LHG	Y	318	25	-	23/47/47/53	-
24	CHL	3	308	-	-	3/14/90/117	-
24	CHL	7	310	-	-	7/17/93/117	-
25	CLA	8	305	17	-	11/26/102/115	-
25	CLA	b	608	-	-	10/27/103/115	-
30	LHG	p	319	25	-	26/47/47/53	-
25	CLA	u	308	-	-	7/21/97/115	-
25	CLA	N	307	-	-	6/21/97/115	-
25	CLA	a	603	19	-	13/39/115/115	-
25	CLA	s	404	-	-	5/15/91/115	-
32	SQD	A	609	-	-	16/40/60/69	0/1/1/1
35	PHO	D	403	-	-	11/37/103/103	0/5/6/6
24	CHL	r	302	8	-	5/17/93/117	-
24	CHL	p	318	12	-	5/12/88/117	-
25	CLA	1	315	10	-	8/15/91/115	-
29	0UR	8	301	-	-	10/42/81/86	0/2/2/2
24	CHL	3	304	12	-	8/20/96/117	-
24	CHL	5	311	-	-	7/19/95/117	-
24	CHL	R	601	8	-	5/17/93/117	-
25	CLA	b	613	18	-	10/39/115/115	-
24	CHL	g	309	-	-	2/14/90/117	-
31	8CT	x	601	-	-	10/29/63/63	0/2/2/2
25	CLA	r	310	8	-	4/27/103/115	-
25	CLA	c	602	20	-	17/39/115/115	-
25	CLA	g	315	-	-	6/33/109/115	-
30	LHG	4	318	-	-	21/46/46/53	-
24	CHL	Y	310	-	-	12/27/103/117	-
28	NEX	y	304	-	-	5/27/83/83	0/3/3/3
33	LMG	B	619	-	-	20/36/56/70	0/1/1/1
24	CHL	s	406	-	-	6/17/93/117	-
25	CLA	B	605	18	-	16/39/115/115	-
28	NEX	3	318	-	-	4/27/83/83	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	G	304	-	-	5/27/83/83	0/3/3/3
24	CHL	5	318	11	-	6/12/88/117	-
24	CHL	n	305	-	-	20/34/110/117	-
26	0IE	u	303	-	-	2/33/72/72	0/2/2/2
29	0UR	p	301	-	-	8/42/81/86	0/2/2/2
25	CLA	Y	307	-	-	9/21/97/115	-
25	CLA	S	609	-	-	5/27/103/115	-
24	CHL	S	606	-	-	6/17/93/117	-
24	CHL	6	305	-	-	12/20/96/117	-
25	CLA	N	306	17	-	10/26/102/115	-
28	NEX	S	617	-	-	5/27/83/83	0/3/3/3
25	CLA	a	605	-	-	8/20/96/115	-
24	CHL	9	304	12	-	15/41/117/117	-
24	CHL	4	311	-	-	3/15/91/117	-
25	CLA	s	411	-	-	4/13/90/115	-
26	0IE	r	315	-	-	1/33/72/72	0/2/2/2
35	PHO	a	606	-	-	7/37/103/103	0/5/6/6
25	CLA	b	606	18	-	18/39/115/115	-
25	CLA	b	603	18	-	12/39/115/115	-
25	CLA	c	610	-	-	9/39/115/115	-
32	SQD	B	618	-	-	16/49/69/69	0/1/1/1
25	CLA	4	307	28	-	4/10/86/115	-
25	CLA	u	317	12	-	8/27/103/115	-
24	CHL	3	310	-	-	7/17/93/117	-
24	CHL	p	312	-	-	7/19/95/117	-
24	CHL	7	318	12	-	5/12/88/117	-
39	PL9	D	406	-	-	13/53/73/73	0/1/1/1
28	NEX	6	303	-	-	4/27/83/83	0/3/3/3
30	LHG	1	318	-	-	23/46/46/53	-
33	LMG	m	101	-	-	19/36/56/70	0/1/1/1
24	CHL	9	305	-	-	17/39/115/117	-
30	LHG	d	408	-	-	25/43/43/53	-
24	CHL	9	310	-	-	4/17/93/117	-
25	CLA	B	604	18	-	16/36/112/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	6	316	-	-	11/15/91/115	-
31	8CT	X	601	-	-	10/29/63/63	0/2/2/2
25	CLA	r	304	-	-	6/18/94/115	-
24	CHL	3	312	-	-	5/14/90/117	-
25	CLA	6	307	-	-	8/13/89/115	-
25	CLA	Y	316	17	-	11/27/103/115	-
24	CHL	8	308	-	-	5/17/93/117	-
25	CLA	1	306	-	-	6/13/90/115	-
25	CLA	q	312	-	-	3/27/103/115	-
32	SQD	a	609	-	-	19/40/60/69	0/1/1/1
31	8CT	D	410	-	-	10/29/63/63	0/2/2/2
24	CHL	p	313	-	-	4/14/90/117	-
28	NEX	n	303	-	-	4/27/83/83	0/3/3/3
25	CLA	G	315	-	-	7/33/109/115	-
25	CLA	Y	313	17	-	5/27/103/115	-
33	LMG	d	411	-	-	21/41/61/70	0/1/1/1
25	CLA	N	313	-	-	5/27/103/115	-
25	CLA	8	314	-	-	5/13/89/115	-
25	CLA	6	314	-	-	4/10/86/115	-
28	NEX	4	303	25	-	5/27/83/83	0/3/3/3
30	LHG	2	319	-	-	20/44/44/53	-

All (6030) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	8CT	C02-C03	14.71	1.59	1.34
31	d	410	8CT	C02-C03	14.58	1.59	1.34
31	S	614	8CT	C02-C03	14.32	1.59	1.34
31	s	415	8CT	C02-C03	14.31	1.59	1.34
31	A	608	8CT	C02-C03	14.29	1.59	1.34
31	a	608	8CT	C02-C03	14.24	1.59	1.34
31	B	617	8CT	C02-C03	14.21	1.59	1.34
31	b	617	8CT	C02-C03	14.19	1.59	1.34
31	x	601	8CT	C02-C03	14.15	1.58	1.34
31	V	401	8CT	C02-C03	14.13	1.58	1.34
31	v	401	8CT	C02-C03	14.13	1.58	1.34
31	X	601	8CT	C02-C03	14.12	1.58	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	615	8CT	C02-C03	14.12	1.58	1.34
31	C	615	8CT	C02-C03	14.11	1.58	1.34
31	c	613	8CT	C02-C03	14.06	1.58	1.34
31	C	613	8CT	C02-C03	14.01	1.58	1.34
31	s	416	8CT	C02-C03	14.00	1.58	1.34
31	T	101	8CT	C02-C03	13.97	1.58	1.34
31	t	101	8CT	C02-C03	13.94	1.58	1.34
31	d	410	8CT	C32-C31	13.92	1.60	1.32
31	D	410	8CT	C32-C31	13.92	1.60	1.32
31	v	401	8CT	C32-C31	13.90	1.60	1.32
31	V	401	8CT	C32-C31	13.90	1.60	1.32
31	S	615	8CT	C02-C03	13.88	1.58	1.34
31	b	617	8CT	C32-C31	13.88	1.60	1.32
31	B	617	8CT	C32-C31	13.81	1.59	1.32
31	X	601	8CT	C32-C31	13.73	1.59	1.32
31	A	608	8CT	C32-C31	13.72	1.59	1.32
31	x	601	8CT	C32-C31	13.72	1.59	1.32
31	a	608	8CT	C32-C31	13.72	1.59	1.32
31	C	613	8CT	C32-C31	13.66	1.59	1.32
31	S	615	8CT	C32-C31	13.65	1.59	1.32
31	c	614	8CT	C32-C31	13.65	1.59	1.32
31	s	416	8CT	C32-C31	13.63	1.59	1.32
31	c	613	8CT	C32-C31	13.63	1.59	1.32
31	C	614	8CT	C32-C31	13.62	1.59	1.32
31	C	614	8CT	C02-C03	13.59	1.58	1.34
31	S	614	8CT	C32-C31	13.58	1.59	1.32
31	s	415	8CT	C32-C31	13.58	1.59	1.32
31	t	101	8CT	C32-C31	13.56	1.59	1.32
31	c	614	8CT	C02-C03	13.54	1.57	1.34
31	c	615	8CT	C32-C31	13.53	1.59	1.32
31	T	101	8CT	C32-C31	13.52	1.59	1.32
31	C	615	8CT	C32-C31	13.52	1.59	1.32
35	d	403	PHO	C1B-C2B	8.87	1.49	1.39
35	D	403	PHO	C1B-C2B	8.74	1.49	1.39
35	A	606	PHO	C1B-C2B	8.60	1.49	1.39
35	a	606	PHO	C1B-C2B	8.58	1.49	1.39
31	X	601	8CT	C34-C35	-8.39	1.36	1.54
31	a	608	8CT	C34-C35	-8.34	1.37	1.54
31	x	601	8CT	C34-C35	-8.33	1.37	1.54
31	A	608	8CT	C34-C35	-8.31	1.37	1.54
31	c	614	8CT	C34-C35	-8.29	1.37	1.54
31	c	613	8CT	C34-C35	-8.28	1.37	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	615	8CT	C34-C35	-8.26	1.37	1.54
31	C	613	8CT	C34-C35	-8.24	1.37	1.54
31	C	614	8CT	C34-C35	-8.23	1.37	1.54
31	c	615	8CT	C34-C35	-8.21	1.37	1.54
31	s	415	8CT	C34-C35	-8.14	1.37	1.54
31	S	614	8CT	C34-C35	-8.10	1.37	1.54
31	v	401	8CT	C34-C35	-7.99	1.37	1.54
31	V	401	8CT	C34-C35	-7.92	1.37	1.54
31	s	416	8CT	C34-C35	-7.86	1.38	1.54
31	d	410	8CT	C34-C35	-7.84	1.38	1.54
31	S	615	8CT	C34-C35	-7.83	1.38	1.54
31	B	617	8CT	C34-C35	-7.83	1.38	1.54
31	D	410	8CT	C34-C35	-7.82	1.38	1.54
31	b	617	8CT	C34-C35	-7.81	1.38	1.54
31	t	101	8CT	C34-C35	-7.75	1.38	1.54
31	T	101	8CT	C34-C35	-7.74	1.38	1.54
35	A	606	PHO	C3B-C4B	7.17	1.49	1.41
35	a	606	PHO	C3B-C4B	7.03	1.49	1.41
31	S	615	8CT	C15-C16	7.01	1.61	1.45
31	s	416	8CT	C15-C16	6.98	1.60	1.45
35	D	403	PHO	C3B-C4B	6.96	1.49	1.41
35	d	403	PHO	C3B-C4B	6.94	1.49	1.41
31	s	415	8CT	C15-C16	6.73	1.60	1.45
31	S	614	8CT	C15-C16	6.69	1.60	1.45
31	T	101	8CT	C05-C06	-6.69	1.36	1.52
31	c	614	8CT	C05-C06	-6.68	1.36	1.52
31	t	101	8CT	C05-C06	-6.67	1.36	1.52
31	C	614	8CT	C05-C06	-6.65	1.36	1.52
31	X	601	8CT	C05-C06	-6.61	1.36	1.52
31	D	410	8CT	C05-C06	-6.60	1.36	1.52
31	A	608	8CT	C05-C06	-6.59	1.36	1.52
31	a	608	8CT	C05-C06	-6.59	1.36	1.52
31	d	410	8CT	C05-C06	-6.58	1.36	1.52
31	x	601	8CT	C05-C06	-6.57	1.36	1.52
31	S	614	8CT	C28-C26	6.54	1.60	1.45
31	c	615	8CT	C05-C06	-6.53	1.36	1.52
31	S	615	8CT	C05-C06	-6.52	1.36	1.52
31	s	416	8CT	C05-C06	-6.52	1.36	1.52
31	s	415	8CT	C28-C26	6.52	1.59	1.45
31	S	614	8CT	C05-C06	-6.51	1.36	1.52
31	s	415	8CT	C05-C06	-6.51	1.36	1.52
31	v	401	8CT	C05-C06	-6.51	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	613	8CT	C05-C06	-6.50	1.36	1.52
31	C	613	8CT	C05-C06	-6.49	1.36	1.52
31	V	401	8CT	C05-C06	-6.48	1.36	1.52
31	C	615	8CT	C05-C06	-6.47	1.36	1.52
31	b	617	8CT	C15-C16	6.32	1.59	1.45
31	B	617	8CT	C05-C06	-6.31	1.37	1.52
31	b	617	8CT	C05-C06	-6.31	1.37	1.52
31	v	401	8CT	C28-C26	6.28	1.59	1.45
31	a	608	8CT	C15-C16	6.27	1.59	1.45
31	C	613	8CT	C15-C16	6.27	1.59	1.45
31	T	101	8CT	C15-C16	6.26	1.59	1.45
31	S	615	8CT	C28-C26	6.25	1.59	1.45
31	s	416	8CT	C28-C26	6.25	1.59	1.45
31	B	617	8CT	C15-C16	6.25	1.59	1.45
31	v	401	8CT	C15-C16	6.25	1.59	1.45
31	c	613	8CT	C15-C16	6.25	1.59	1.45
31	C	615	8CT	C15-C16	6.24	1.59	1.45
31	V	401	8CT	C28-C26	6.24	1.59	1.45
31	V	401	8CT	C15-C16	6.23	1.59	1.45
31	c	615	8CT	C15-C16	6.23	1.59	1.45
31	d	410	8CT	C28-C26	6.23	1.59	1.45
31	t	101	8CT	C15-C16	6.22	1.59	1.45
31	D	410	8CT	C28-C26	6.21	1.59	1.45
31	d	410	8CT	C15-C16	6.20	1.59	1.45
31	X	601	8CT	C15-C16	6.20	1.59	1.45
31	D	410	8CT	C15-C16	6.20	1.59	1.45
31	A	608	8CT	C15-C16	6.19	1.59	1.45
31	C	614	8CT	C15-C16	6.16	1.59	1.45
31	x	601	8CT	C15-C16	6.15	1.59	1.45
31	t	101	8CT	C28-C26	6.15	1.59	1.45
31	c	614	8CT	C15-C16	6.14	1.59	1.45
31	b	617	8CT	C28-C26	6.13	1.59	1.45
31	T	101	8CT	C28-C26	6.11	1.59	1.45
31	B	617	8CT	C28-C26	6.08	1.59	1.45
31	C	613	8CT	C28-C26	6.07	1.59	1.45
31	X	601	8CT	C28-C26	6.02	1.58	1.45
31	c	613	8CT	C28-C26	6.01	1.58	1.45
31	x	601	8CT	C28-C26	6.00	1.58	1.45
31	s	416	8CT	C23-C21	5.98	1.58	1.45
31	S	615	8CT	C23-C21	5.95	1.58	1.45
31	C	614	8CT	C28-C26	5.95	1.58	1.45
39	d	406	PL9	C7-C3	-5.95	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	614	8CT	C28-C26	5.91	1.58	1.45
31	A	608	8CT	C28-C26	5.86	1.58	1.45
31	a	608	8CT	C28-C26	5.85	1.58	1.45
39	D	406	PL9	C7-C3	-5.85	1.45	1.51
31	C	615	8CT	C28-C26	5.83	1.58	1.45
31	c	615	8CT	C04-C03	-5.81	1.45	1.53
31	c	615	8CT	C28-C26	5.81	1.58	1.45
31	C	614	8CT	C04-C03	-5.79	1.45	1.53
31	c	614	8CT	C04-C03	-5.78	1.45	1.53
31	C	615	8CT	C04-C03	-5.77	1.45	1.53
31	t	101	8CT	C23-C21	5.73	1.58	1.45
31	T	101	8CT	C23-C21	5.73	1.58	1.45
31	S	614	8CT	C23-C21	5.70	1.58	1.45
31	V	401	8CT	C23-C21	5.70	1.58	1.45
31	b	617	8CT	C23-C21	5.69	1.58	1.45
31	v	401	8CT	C23-C21	5.69	1.58	1.45
31	A	608	8CT	C04-C03	-5.69	1.46	1.53
31	D	410	8CT	C23-C21	5.66	1.58	1.45
31	s	415	8CT	C23-C21	5.66	1.58	1.45
31	b	617	8CT	C34-C33	5.64	1.65	1.52
31	B	617	8CT	C34-C33	5.64	1.65	1.52
31	B	617	8CT	C23-C21	5.63	1.58	1.45
31	a	608	8CT	C04-C03	-5.63	1.46	1.53
31	T	101	8CT	C34-C33	5.63	1.65	1.52
31	t	101	8CT	C34-C33	5.63	1.65	1.52
31	s	416	8CT	C04-C03	-5.61	1.46	1.53
31	d	410	8CT	C23-C21	5.60	1.58	1.45
31	v	401	8CT	C04-C03	-5.59	1.46	1.53
31	S	615	8CT	C04-C03	-5.56	1.46	1.53
31	V	401	8CT	C04-C03	-5.56	1.46	1.53
31	T	101	8CT	C04-C03	-5.56	1.46	1.53
31	c	615	8CT	C23-C21	5.55	1.57	1.45
31	D	410	8CT	C34-C33	5.55	1.65	1.52
31	d	410	8CT	C34-C33	5.54	1.65	1.52
31	C	613	8CT	C23-C21	5.54	1.57	1.45
31	C	615	8CT	C23-C21	5.52	1.57	1.45
31	c	613	8CT	C23-C21	5.52	1.57	1.45
31	t	101	8CT	C04-C03	-5.52	1.46	1.53
31	X	601	8CT	C04-C03	-5.51	1.46	1.53
31	x	601	8CT	C23-C21	5.50	1.57	1.45
31	X	601	8CT	C23-C21	5.50	1.57	1.45
31	x	601	8CT	C04-C03	-5.48	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	410	8CT	C04-C03	-5.47	1.46	1.53
31	c	613	8CT	C04-C03	-5.46	1.46	1.53
31	s	416	8CT	C34-C33	5.44	1.65	1.52
31	s	415	8CT	C34-C33	5.43	1.65	1.52
31	v	401	8CT	C34-C33	5.43	1.65	1.52
31	V	401	8CT	C34-C33	5.42	1.65	1.52
31	C	613	8CT	C04-C03	-5.41	1.46	1.53
31	S	615	8CT	C34-C33	5.41	1.65	1.52
31	c	614	8CT	C23-C21	5.41	1.57	1.45
31	C	614	8CT	C23-C21	5.40	1.57	1.45
31	S	614	8CT	C34-C33	5.40	1.65	1.52
31	b	617	8CT	C04-C03	-5.34	1.46	1.53
31	D	410	8CT	C04-C03	-5.33	1.46	1.53
31	c	614	8CT	C34-C33	5.32	1.65	1.52
31	C	614	8CT	C34-C33	5.31	1.65	1.52
31	s	415	8CT	C04-C03	-5.28	1.46	1.53
31	a	608	8CT	C23-C21	5.27	1.57	1.45
31	S	614	8CT	C04-C03	-5.26	1.46	1.53
31	A	608	8CT	C23-C21	5.26	1.57	1.45
24	R	601	CHL	O2D-CGD	5.25	1.46	1.33
31	a	608	8CT	C34-C33	5.24	1.64	1.52
31	B	617	8CT	C04-C03	-5.23	1.46	1.53
31	C	615	8CT	C34-C33	5.22	1.64	1.52
31	x	601	8CT	C34-C33	5.22	1.64	1.52
31	B	617	8CT	C05-C04	5.22	1.66	1.54
31	A	608	8CT	C34-C33	5.22	1.64	1.52
31	c	613	8CT	C34-C33	5.22	1.64	1.52
24	r	302	CHL	O2D-CGD	5.22	1.45	1.33
31	b	617	8CT	C05-C04	5.21	1.66	1.54
24	G	309	CHL	O2D-CGD	5.21	1.45	1.33
31	X	601	8CT	C34-C33	5.21	1.64	1.52
24	4	317	CHL	O2D-CGD	5.21	1.45	1.33
24	1	317	CHL	O2D-CGD	5.21	1.45	1.33
31	c	615	8CT	C34-C33	5.20	1.64	1.52
24	g	309	CHL	O2D-CGD	5.20	1.45	1.33
24	8	315	CHL	O2D-CGD	5.20	1.45	1.33
24	9	317	CHL	O2D-CGD	5.19	1.45	1.33
24	q	316	CHL	O2D-CGD	5.19	1.45	1.33
31	C	613	8CT	C34-C33	5.19	1.64	1.52
24	u	310	CHL	O2D-CGD	5.19	1.45	1.33
24	3	308	CHL	O2D-CGD	5.18	1.45	1.33
24	4	304	CHL	O2D-CGD	5.18	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	317	CHL	O2D-CGD	5.18	1.45	1.33
24	9	311	CHL	O2D-CGD	5.17	1.45	1.33
24	u	318	CHL	O2D-CGD	5.17	1.45	1.33
24	6	308	CHL	O2D-CGD	5.17	1.45	1.33
24	u	306	CHL	O2D-CGD	5.17	1.45	1.33
24	u	309	CHL	O2D-CGD	5.16	1.45	1.33
24	9	310	CHL	O2D-CGD	5.16	1.45	1.33
24	u	311	CHL	O2D-CGD	5.16	1.45	1.33
24	1	304	CHL	O2D-CGD	5.16	1.45	1.33
24	n	309	CHL	O2D-CGD	5.16	1.45	1.33
24	9	308	CHL	O2D-CGD	5.16	1.45	1.33
24	6	310	CHL	O2D-CGD	5.15	1.45	1.33
24	6	311	CHL	O2D-CGD	5.15	1.45	1.33
24	9	309	CHL	O2D-CGD	5.15	1.45	1.33
24	G	310	CHL	O2D-CGD	5.15	1.45	1.33
24	u	312	CHL	O2D-CGD	5.15	1.45	1.33
24	6	305	CHL	O2D-CGD	5.15	1.45	1.33
24	N	305	CHL	O2D-CGD	5.14	1.45	1.33
24	1	308	CHL	O2D-CGD	5.14	1.45	1.33
24	1	305	CHL	O2D-CGD	5.14	1.45	1.33
24	N	317	CHL	O2D-CGD	5.14	1.45	1.33
24	9	305	CHL	O2D-CGD	5.14	1.45	1.33
24	3	305	CHL	O2D-CGD	5.14	1.45	1.33
24	N	304	CHL	O2D-CGD	5.14	1.45	1.33
24	4	305	CHL	O2D-CGD	5.14	1.45	1.33
24	g	310	CHL	O2D-CGD	5.14	1.45	1.33
24	N	311	CHL	O2D-CGD	5.14	1.45	1.33
24	7	309	CHL	O2D-CGD	5.14	1.45	1.33
24	3	310	CHL	O2D-CGD	5.14	1.45	1.33
24	n	304	CHL	O2D-CGD	5.14	1.45	1.33
24	4	308	CHL	O2D-CGD	5.14	1.45	1.33
24	g	312	CHL	O2D-CGD	5.13	1.45	1.33
24	g	311	CHL	O2D-CGD	5.13	1.45	1.33
24	1	311	CHL	O2D-CGD	5.13	1.45	1.33
24	u	309	CHL	C2C-C3C	5.13	1.47	1.36
24	3	309	CHL	O2D-CGD	5.13	1.45	1.33
24	N	309	CHL	O2D-CGD	5.13	1.45	1.33
24	n	311	CHL	O2D-CGD	5.12	1.45	1.33
24	6	309	CHL	O2D-CGD	5.12	1.45	1.33
24	u	305	CHL	O2D-CGD	5.12	1.45	1.33
24	n	305	CHL	O2D-CGD	5.12	1.45	1.33
24	9	308	CHL	C2C-C3C	5.12	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	311	CHL	O2D-CGD	5.12	1.45	1.33
24	5	311	CHL	O2D-CGD	5.12	1.45	1.33
24	9	312	CHL	O2D-CGD	5.12	1.45	1.33
24	N	312	CHL	O2D-CGD	5.12	1.45	1.33
24	3	311	CHL	O2D-CGD	5.11	1.45	1.33
24	G	312	CHL	O2D-CGD	5.11	1.45	1.33
24	3	317	CHL	O2D-CGD	5.11	1.45	1.33
24	s	407	CHL	O2D-CGD	5.11	1.45	1.33
24	G	306	CHL	O2D-CGD	5.11	1.45	1.33
24	9	317	CHL	CHD-C1D	5.11	1.48	1.38
24	g	305	CHL	O2D-CGD	5.11	1.45	1.33
24	p	309	CHL	O2D-CGD	5.11	1.45	1.33
24	r	306	CHL	O2D-CGD	5.11	1.45	1.33
24	n	308	CHL	O2D-CGD	5.11	1.45	1.33
24	Y	309	CHL	O2D-CGD	5.11	1.45	1.33
24	5	310	CHL	O2D-CGD	5.11	1.45	1.33
24	y	310	CHL	O2D-CGD	5.10	1.45	1.33
24	u	318	CHL	CHD-C1D	5.10	1.48	1.38
24	2	311	CHL	O2D-CGD	5.10	1.45	1.33
24	6	317	CHL	O2D-CGD	5.10	1.45	1.33
24	u	313	CHL	O2D-CGD	5.10	1.45	1.33
24	2	310	CHL	O2D-CGD	5.10	1.45	1.33
24	4	309	CHL	O2D-CGD	5.10	1.45	1.33
24	n	312	CHL	O2D-CGD	5.10	1.45	1.33
24	9	317	CHL	C2C-C3C	5.09	1.47	1.36
24	2	305	CHL	O2D-CGD	5.09	1.45	1.33
24	N	310	CHL	O2D-CGD	5.09	1.45	1.33
24	p	318	CHL	O2D-CGD	5.09	1.45	1.33
24	G	309	CHL	C2C-C3C	5.09	1.47	1.36
24	p	309	CHL	C2C-C3C	5.09	1.47	1.36
24	S	606	CHL	O2D-CGD	5.09	1.45	1.33
24	9	304	CHL	O2D-CGD	5.09	1.45	1.33
24	n	310	CHL	O2D-CGD	5.09	1.45	1.33
24	s	406	CHL	O2D-CGD	5.09	1.45	1.33
24	u	318	CHL	C2C-C3C	5.09	1.47	1.36
24	g	313	CHL	O2D-CGD	5.09	1.45	1.33
31	c	613	8CT	C05-C04	5.09	1.65	1.54
24	4	310	CHL	O2D-CGD	5.09	1.45	1.33
24	6	312	CHL	O2D-CGD	5.09	1.45	1.33
24	g	306	CHL	O2D-CGD	5.09	1.45	1.33
24	2	313	CHL	O2D-CGD	5.09	1.45	1.33
24	p	310	CHL	O2D-CGD	5.09	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	310	CHL	O2D-CGD	5.08	1.45	1.33
24	1	317	CHL	C2C-C3C	5.08	1.47	1.36
24	3	304	CHL	O2D-CGD	5.08	1.45	1.33
24	G	313	CHL	O2D-CGD	5.08	1.45	1.33
24	1	310	CHL	O2D-CGD	5.08	1.45	1.33
24	5	313	CHL	O2D-CGD	5.08	1.45	1.33
24	R	605	CHL	O2D-CGD	5.07	1.45	1.33
24	y	309	CHL	O2D-CGD	5.07	1.45	1.33
24	Y	308	CHL	O2D-CGD	5.07	1.45	1.33
24	p	311	CHL	O2D-CGD	5.07	1.45	1.33
24	g	309	CHL	C2C-C3C	5.07	1.47	1.36
24	p	309	CHL	CHD-C1D	5.07	1.48	1.38
31	S	614	8CT	C05-C04	5.07	1.65	1.54
24	y	311	CHL	O2D-CGD	5.07	1.45	1.33
24	R	606	CHL	O2D-CGD	5.07	1.45	1.33
24	3	312	CHL	O2D-CGD	5.07	1.45	1.33
24	5	312	CHL	O2D-CGD	5.06	1.45	1.33
31	s	415	8CT	C05-C04	5.06	1.65	1.54
24	G	305	CHL	O2D-CGD	5.06	1.45	1.33
24	G	311	CHL	O2D-CGD	5.06	1.45	1.33
31	C	613	8CT	C05-C04	5.06	1.65	1.54
24	1	309	CHL	O2D-CGD	5.06	1.45	1.33
24	7	318	CHL	O2D-CGD	5.06	1.45	1.33
24	5	305	CHL	O2D-CGD	5.06	1.45	1.33
24	3	312	CHL	C2C-C3C	5.06	1.47	1.36
24	n	317	CHL	C2C-C3C	5.06	1.47	1.36
24	p	312	CHL	O2D-CGD	5.05	1.45	1.33
24	Y	310	CHL	O2D-CGD	5.05	1.45	1.33
24	g	309	CHL	CHD-C1D	5.05	1.48	1.38
24	7	309	CHL	CHD-C1D	5.05	1.48	1.38
24	6	304	CHL	O2D-CGD	5.05	1.45	1.33
24	7	309	CHL	C2C-C3C	5.05	1.47	1.36
24	N	317	CHL	C2C-C3C	5.05	1.47	1.36
24	5	309	CHL	O2D-CGD	5.05	1.45	1.33
24	N	308	CHL	O2D-CGD	5.04	1.45	1.33
24	5	318	CHL	O2D-CGD	5.04	1.45	1.33
24	n	317	CHL	CHD-C1D	5.04	1.48	1.38
24	4	317	CHL	C2C-C3C	5.04	1.47	1.36
24	r	307	CHL	O2D-CGD	5.04	1.45	1.33
24	1	304	CHL	C2C-C3C	5.04	1.47	1.36
24	3	309	CHL	C2C-C3C	5.04	1.47	1.36
24	2	318	CHL	O2D-CGD	5.04	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	313	CHL	C2C-C3C	5.04	1.47	1.36
24	2	312	CHL	O2D-CGD	5.04	1.45	1.33
24	S	605	CHL	O2D-CGD	5.04	1.45	1.33
24	g	318	CHL	O2D-CGD	5.03	1.45	1.33
24	Y	319	CHL	O2D-CGD	5.03	1.45	1.33
24	7	311	CHL	O2D-CGD	5.03	1.45	1.33
24	R	607	CHL	O2D-CGD	5.03	1.45	1.33
24	q	309	CHL	O2D-CGD	5.03	1.45	1.33
24	s	408	CHL	O2D-CGD	5.03	1.45	1.33
24	4	304	CHL	C2C-C3C	5.03	1.47	1.36
24	u	313	CHL	C2C-C3C	5.03	1.47	1.36
24	2	309	CHL	O2D-CGD	5.03	1.45	1.33
24	g	313	CHL	C2C-C3C	5.02	1.47	1.36
24	s	409	CHL	O2D-CGD	5.02	1.45	1.33
24	r	308	CHL	O2D-CGD	5.02	1.45	1.33
24	G	309	CHL	CHD-C1D	5.02	1.48	1.38
24	1	312	CHL	O2D-CGD	5.02	1.45	1.33
24	S	607	CHL	O2D-CGD	5.02	1.45	1.33
24	G	318	CHL	O2D-CGD	5.02	1.45	1.33
24	1	317	CHL	CHD-C1D	5.02	1.48	1.38
24	N	317	CHL	CHD-C1D	5.02	1.48	1.38
24	9	312	CHL	C2C-C3C	5.01	1.47	1.36
24	3	312	CHL	CHD-C1D	5.01	1.48	1.38
24	q	304	CHL	O2D-CGD	5.01	1.45	1.33
24	6	312	CHL	C2C-C3C	5.01	1.47	1.36
24	R	608	CHL	O2D-CGD	5.01	1.45	1.33
24	S	608	CHL	O2D-CGD	5.01	1.45	1.33
24	7	312	CHL	O2D-CGD	5.01	1.45	1.33
24	5	306	CHL	O2D-CGD	5.01	1.45	1.33
31	x	601	8CT	C05-C04	5.01	1.65	1.54
24	6	309	CHL	C2C-C3C	5.00	1.47	1.36
24	4	317	CHL	CHD-C1D	5.00	1.48	1.38
24	R	601	CHL	C2C-C3C	5.00	1.47	1.36
24	g	313	CHL	CHD-C1D	5.00	1.48	1.38
24	4	308	CHL	C2C-C3C	5.00	1.47	1.36
24	4	312	CHL	O2D-CGD	5.00	1.45	1.33
24	S	602	CHL	O2D-CGD	5.00	1.45	1.33
24	s	403	CHL	O2D-CGD	5.00	1.45	1.33
24	3	308	CHL	C2C-C3C	5.00	1.47	1.36
31	X	601	8CT	C05-C04	4.99	1.65	1.54
24	q	303	CHL	O2D-CGD	4.99	1.45	1.33
24	9	308	CHL	CHD-C1D	4.99	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	308	CHL	C2C-C3C	4.99	1.47	1.36
24	q	308	CHL	O2D-CGD	4.99	1.45	1.33
24	u	305	CHL	C2C-C3C	4.99	1.47	1.36
24	G	313	CHL	CHD-C1D	4.99	1.48	1.38
24	u	313	CHL	CHD-C1D	4.99	1.48	1.38
24	1	304	CHL	CHD-C1D	4.98	1.48	1.38
24	8	315	CHL	C2C-C3C	4.98	1.47	1.36
24	q	316	CHL	C2C-C3C	4.98	1.47	1.36
24	Y	312	CHL	O2D-CGD	4.98	1.45	1.33
24	8	304	CHL	O2D-CGD	4.98	1.45	1.33
24	6	308	CHL	C2C-C3C	4.98	1.47	1.36
24	8	308	CHL	O2D-CGD	4.98	1.45	1.33
24	9	312	CHL	CHD-C1D	4.98	1.48	1.38
24	p	313	CHL	O2D-CGD	4.98	1.45	1.33
24	2	306	CHL	O2D-CGD	4.97	1.45	1.33
24	3	308	CHL	CHD-C1D	4.97	1.48	1.38
24	R	602	CHL	O2D-CGD	4.97	1.45	1.33
24	9	310	CHL	C2C-C3C	4.97	1.47	1.36
24	6	312	CHL	CHD-C1D	4.97	1.48	1.38
24	7	313	CHL	O2D-CGD	4.96	1.45	1.33
24	r	309	CHL	O2D-CGD	4.96	1.45	1.33
24	p	305	CHL	O2D-CGD	4.96	1.45	1.33
24	7	306	CHL	O2D-CGD	4.96	1.45	1.33
24	8	303	CHL	O2D-CGD	4.96	1.45	1.33
24	8	307	CHL	O2D-CGD	4.96	1.45	1.33
24	7	305	CHL	O2D-CGD	4.95	1.45	1.33
24	Y	317	CHL	O2D-CGD	4.95	1.45	1.33
31	d	410	8CT	C05-C04	4.95	1.65	1.54
24	u	305	CHL	CHD-C1D	4.95	1.48	1.38
24	q	316	CHL	CHD-C1D	4.95	1.48	1.38
31	s	416	8CT	C05-C04	4.95	1.65	1.54
24	q	310	CHL	O2D-CGD	4.95	1.45	1.33
31	S	615	8CT	C05-C04	4.95	1.65	1.54
24	1	309	CHL	C2C-C3C	4.95	1.47	1.36
24	y	313	CHL	O2D-CGD	4.95	1.45	1.33
24	y	306	CHL	O2D-CGD	4.94	1.45	1.33
24	r	303	CHL	O2D-CGD	4.94	1.45	1.33
24	8	310	CHL	O2D-CGD	4.94	1.45	1.33
24	4	304	CHL	CHD-C1D	4.94	1.48	1.38
24	8	315	CHL	CHD-C1D	4.94	1.48	1.38
24	p	306	CHL	O2D-CGD	4.94	1.45	1.33
24	u	311	CHL	C2C-C3C	4.94	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	310	CHL	C2C-C3C	4.93	1.47	1.36
24	4	308	CHL	CHD-C1D	4.93	1.48	1.38
24	s	402	CHL	O2D-CGD	4.93	1.45	1.33
24	6	308	CHL	CHD-C1D	4.93	1.48	1.38
24	q	307	CHL	O2D-CGD	4.93	1.45	1.33
24	s	414	CHL	C3A-C2A	-4.93	1.49	1.54
24	q	311	CHL	O2D-CGD	4.92	1.45	1.33
24	u	309	CHL	CHD-C1D	4.92	1.47	1.38
31	D	410	8CT	C05-C04	4.92	1.65	1.54
24	y	318	CHL	O2D-CGD	4.92	1.45	1.33
24	u	310	CHL	C2C-C3C	4.91	1.47	1.36
24	8	303	CHL	CHD-C1D	4.91	1.47	1.38
24	4	309	CHL	C2C-C3C	4.91	1.47	1.36
24	Y	305	CHL	O2D-CGD	4.91	1.45	1.33
24	y	312	CHL	O2D-CGD	4.91	1.45	1.33
24	3	310	CHL	C2C-C3C	4.91	1.47	1.36
24	5	309	CHL	C2C-C3C	4.91	1.47	1.36
24	Y	311	CHL	O2D-CGD	4.90	1.45	1.33
24	8	309	CHL	O2D-CGD	4.90	1.45	1.33
24	r	302	CHL	C2C-C3C	4.90	1.47	1.36
31	v	401	8CT	C05-C04	4.90	1.65	1.54
24	n	304	CHL	C2C-C3C	4.90	1.47	1.36
24	n	308	CHL	C2C-C3C	4.90	1.47	1.36
24	S	601	CHL	O2D-CGD	4.89	1.45	1.33
24	6	310	CHL	CHD-C1D	4.89	1.47	1.38
24	g	310	CHL	CHD-C1D	4.89	1.47	1.38
24	1	308	CHL	CHD-C1D	4.89	1.47	1.38
24	6	317	CHL	C2C-C3C	4.89	1.47	1.36
31	T	101	8CT	C05-C04	4.89	1.65	1.54
24	S	613	CHL	C3A-C2A	-4.89	1.50	1.54
24	2	318	CHL	C2C-C3C	4.89	1.47	1.36
24	N	304	CHL	C2C-C3C	4.89	1.47	1.36
31	V	401	8CT	C05-C04	4.88	1.65	1.54
24	G	310	CHL	CHD-C1D	4.88	1.47	1.38
24	3	317	CHL	C2C-C3C	4.88	1.47	1.36
24	5	318	CHL	C2C-C3C	4.88	1.47	1.36
24	2	309	CHL	C2C-C3C	4.88	1.47	1.36
24	6	304	CHL	C2C-C3C	4.88	1.47	1.36
24	n	304	CHL	CHD-C1D	4.88	1.47	1.38
24	N	310	CHL	C2C-C3C	4.88	1.47	1.36
24	n	310	CHL	C2C-C3C	4.88	1.47	1.36
24	s	414	CHL	O2D-CGD	4.88	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	613	CHL	O2D-CGD	4.87	1.45	1.33
24	N	308	CHL	C2C-C3C	4.87	1.47	1.36
31	t	101	8CT	C05-C04	4.87	1.65	1.54
24	3	310	CHL	CHD-C1D	4.87	1.47	1.38
24	9	309	CHL	C2C-C3C	4.87	1.47	1.36
24	g	311	CHL	C2C-C3C	4.87	1.47	1.36
24	9	304	CHL	C2C-C3C	4.86	1.47	1.36
24	g	312	CHL	C2C-C3C	4.86	1.47	1.36
24	5	309	CHL	CHD-C1D	4.86	1.47	1.38
24	g	310	CHL	C2C-C3C	4.86	1.47	1.36
24	y	305	CHL	O2D-CGD	4.86	1.45	1.33
24	N	304	CHL	CHD-C1D	4.86	1.47	1.38
24	G	312	CHL	C2C-C3C	4.86	1.47	1.36
24	9	310	CHL	CHD-C1D	4.85	1.47	1.38
24	4	309	CHL	CHD-C1D	4.85	1.47	1.38
24	q	303	CHL	CHD-C1D	4.85	1.47	1.38
24	5	311	CHL	C2C-C3C	4.84	1.47	1.36
31	C	615	8CT	C05-C04	4.84	1.65	1.54
24	9	304	CHL	CHD-C1D	4.84	1.47	1.38
24	G	311	CHL	C2C-C3C	4.84	1.47	1.36
31	a	608	8CT	C05-C04	4.83	1.65	1.54
24	1	309	CHL	CHD-C1D	4.83	1.47	1.38
24	G	310	CHL	C2C-C3C	4.83	1.47	1.36
31	A	608	8CT	C05-C04	4.83	1.65	1.54
31	c	615	8CT	C05-C04	4.83	1.65	1.54
24	N	310	CHL	CHD-C1D	4.82	1.47	1.38
24	3	317	CHL	CHD-C1D	4.82	1.47	1.38
24	n	310	CHL	CHD-C1D	4.82	1.47	1.38
24	2	318	CHL	CHD-C1D	4.82	1.47	1.38
24	4	311	CHL	C2C-C3C	4.81	1.47	1.36
24	2	309	CHL	CHD-C1D	4.81	1.47	1.38
24	Y	304	CHL	O2D-CGD	4.81	1.44	1.33
24	p	310	CHL	C2C-C3C	4.81	1.47	1.36
24	y	318	CHL	C3A-C2A	-4.81	1.50	1.54
24	5	318	CHL	CHD-C1D	4.81	1.47	1.38
24	4	312	CHL	C2C-C3C	4.80	1.47	1.36
24	3	304	CHL	C2C-C3C	4.80	1.47	1.36
24	6	317	CHL	CHD-C1D	4.80	1.47	1.38
24	u	311	CHL	CHD-C1D	4.80	1.47	1.38
24	g	311	CHL	CHD-C1D	4.80	1.47	1.38
29	3	301	0UR	O44-C45	4.80	1.45	1.34
24	6	304	CHL	CHD-C1D	4.80	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	310	CHL	C2C-C3C	4.80	1.47	1.36
24	2	311	CHL	C2C-C3C	4.79	1.47	1.36
24	n	308	CHL	CHD-C1D	4.79	1.47	1.38
24	4	312	CHL	CHD-C1D	4.79	1.47	1.38
24	9	311	CHL	C2C-C3C	4.79	1.47	1.36
24	G	311	CHL	CHD-C1D	4.79	1.47	1.38
24	S	608	CHL	C2C-C3C	4.78	1.47	1.36
29	G	301	0UR	O44-C45	4.78	1.45	1.34
24	s	409	CHL	C2C-C3C	4.78	1.47	1.36
24	8	303	CHL	C2C-C3C	4.78	1.47	1.36
31	c	614	8CT	C05-C04	4.77	1.65	1.54
24	G	312	CHL	CHD-C1D	4.77	1.47	1.38
24	u	310	CHL	CHD-C1D	4.77	1.47	1.38
29	4	301	0UR	O44-C45	4.77	1.45	1.34
31	C	614	8CT	C05-C04	4.77	1.65	1.54
24	9	305	CHL	C2C-C3C	4.77	1.47	1.36
29	Y	301	0UR	O44-C45	4.76	1.45	1.34
29	1	301	0UR	O44-C45	4.76	1.45	1.34
29	N	301	0UR	O44-C45	4.76	1.45	1.34
24	r	309	CHL	C2C-C3C	4.76	1.47	1.36
24	2	311	CHL	CHD-C1D	4.76	1.47	1.38
24	7	318	CHL	C2C-C3C	4.76	1.47	1.36
24	u	312	CHL	C2C-C3C	4.76	1.47	1.36
24	2	305	CHL	C2C-C3C	4.76	1.46	1.36
24	3	309	CHL	CHD-C1D	4.76	1.47	1.38
29	6	301	0UR	O44-C45	4.76	1.45	1.34
29	u	301	0UR	O44-C45	4.76	1.45	1.34
29	n	301	0UR	O44-C45	4.76	1.45	1.34
24	1	311	CHL	C2C-C3C	4.76	1.46	1.36
24	N	308	CHL	CHD-C1D	4.76	1.47	1.38
24	1	312	CHL	C2C-C3C	4.75	1.46	1.36
24	1	312	CHL	CHD-C1D	4.75	1.47	1.38
24	3	311	CHL	C2C-C3C	4.75	1.46	1.36
24	6	311	CHL	C2C-C3C	4.75	1.46	1.36
24	q	303	CHL	C2C-C3C	4.75	1.46	1.36
24	2	313	CHL	CHD-C1D	4.75	1.47	1.38
24	Y	317	CHL	C3A-C2A	-4.75	1.50	1.54
29	g	301	0UR	O44-C45	4.75	1.45	1.34
29	9	301	0UR	O44-C45	4.75	1.45	1.34
24	5	313	CHL	CHD-C1D	4.75	1.47	1.38
29	y	301	0UR	O44-C45	4.75	1.45	1.34
24	R	608	CHL	C2C-C3C	4.75	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	305	CHL	C2C-C3C	4.74	1.46	1.36
24	r	306	CHL	C2C-C3C	4.74	1.46	1.36
24	1	310	CHL	C2C-C3C	4.74	1.46	1.36
24	6	309	CHL	CHD-C1D	4.74	1.47	1.38
24	p	318	CHL	C2C-C3C	4.74	1.46	1.36
24	5	311	CHL	CHD-C1D	4.73	1.47	1.38
24	5	305	CHL	C2C-C3C	4.73	1.46	1.36
24	2	313	CHL	C2C-C3C	4.73	1.46	1.36
24	5	313	CHL	C2C-C3C	4.73	1.46	1.36
24	Y	308	CHL	CHD-C1D	4.73	1.47	1.38
24	u	312	CHL	CHD-C1D	4.73	1.47	1.38
24	g	305	CHL	C2C-C3C	4.72	1.46	1.36
24	g	312	CHL	CHD-C1D	4.72	1.47	1.38
24	u	306	CHL	C2C-C3C	4.72	1.46	1.36
29	7	301	0UR	O44-C45	4.71	1.45	1.34
24	N	312	CHL	C2C-C3C	4.71	1.46	1.36
24	7	310	CHL	CHD-C1D	4.71	1.47	1.38
24	7	313	CHL	CHD-C1D	4.71	1.47	1.38
24	Y	308	CHL	C2C-C3C	4.71	1.46	1.36
24	2	305	CHL	CHD-C1D	4.71	1.47	1.38
24	n	312	CHL	CHD-C1D	4.71	1.47	1.38
24	R	601	CHL	CHD-C1D	4.71	1.47	1.38
24	G	305	CHL	CHD-C1D	4.70	1.47	1.38
24	N	312	CHL	CHD-C1D	4.70	1.47	1.38
24	3	304	CHL	CHD-C1D	4.70	1.47	1.38
24	4	310	CHL	C2C-C3C	4.70	1.46	1.36
24	S	606	CHL	C2C-C3C	4.70	1.46	1.36
24	y	309	CHL	C2C-C3C	4.70	1.46	1.36
24	s	406	CHL	CHD-C1D	4.69	1.47	1.38
24	9	309	CHL	CHD-C1D	4.69	1.47	1.38
24	R	606	CHL	C2C-C3C	4.69	1.46	1.36
24	n	312	CHL	C2C-C3C	4.69	1.46	1.36
24	p	313	CHL	CHD-C1D	4.69	1.47	1.38
24	G	306	CHL	C2C-C3C	4.68	1.46	1.36
24	8	307	CHL	C2C-C3C	4.68	1.46	1.36
24	g	305	CHL	CHD-C1D	4.68	1.47	1.38
24	3	305	CHL	CHD-C1D	4.68	1.47	1.38
24	4	311	CHL	CHD-C1D	4.68	1.47	1.38
24	s	407	CHL	C2C-C3C	4.68	1.46	1.36
24	1	305	CHL	C2C-C3C	4.68	1.46	1.36
24	p	311	CHL	C2C-C3C	4.68	1.46	1.36
24	q	307	CHL	C2C-C3C	4.68	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	307	CHL	C2C-C3C	4.68	1.46	1.36
24	2	312	CHL	C2C-C3C	4.68	1.46	1.36
24	S	606	CHL	CHD-C1D	4.67	1.47	1.38
24	p	313	CHL	C2C-C3C	4.67	1.46	1.36
24	7	313	CHL	C2C-C3C	4.67	1.46	1.36
24	5	305	CHL	CHD-C1D	4.67	1.47	1.38
29	p	301	0UR	O44-C45	4.67	1.45	1.34
24	r	302	CHL	CHD-C1D	4.67	1.47	1.38
24	p	310	CHL	CHD-C1D	4.67	1.47	1.38
24	4	305	CHL	C2C-C3C	4.67	1.46	1.36
24	7	311	CHL	C2C-C3C	4.67	1.46	1.36
24	9	311	CHL	CHD-C1D	4.67	1.47	1.38
24	7	318	CHL	CHD-C1D	4.67	1.47	1.38
24	r	306	CHL	CHD-C1D	4.67	1.47	1.38
24	N	311	CHL	C2C-C3C	4.66	1.46	1.36
24	G	318	CHL	C2C-C3C	4.65	1.46	1.36
24	g	306	CHL	C2C-C3C	4.65	1.46	1.36
29	8	301	0UR	O44-C45	4.65	1.45	1.34
39	D	406	PL9	C3-C4	-4.65	1.41	1.49
24	5	312	CHL	C2C-C3C	4.65	1.46	1.36
29	2	301	0UR	O44-C45	4.64	1.45	1.34
24	3	305	CHL	C2C-C3C	4.64	1.46	1.36
24	9	305	CHL	CHD-C1D	4.64	1.47	1.38
24	g	318	CHL	C2C-C3C	4.64	1.46	1.36
24	p	318	CHL	CHD-C1D	4.64	1.47	1.38
24	6	305	CHL	C2C-C3C	4.64	1.46	1.36
24	y	309	CHL	CHD-C1D	4.64	1.47	1.38
24	n	305	CHL	C2C-C3C	4.63	1.46	1.36
24	1	311	CHL	CHD-C1D	4.63	1.47	1.38
24	g	318	CHL	CHD-C1D	4.63	1.47	1.38
24	S	608	CHL	CHD-C1D	4.63	1.47	1.38
24	4	310	CHL	CHD-C1D	4.63	1.47	1.38
24	n	311	CHL	C2C-C3C	4.62	1.46	1.36
24	N	305	CHL	C2C-C3C	4.62	1.46	1.36
24	9	317	CHL	CHC-C1C	4.62	1.47	1.38
24	s	409	CHL	CHD-C1D	4.62	1.47	1.38
24	s	407	CHL	CHD-C1D	4.62	1.47	1.38
29	5	301	0UR	O44-C45	4.62	1.45	1.34
29	q	301	0UR	O44-C45	4.61	1.45	1.34
24	6	305	CHL	CHD-C1D	4.61	1.47	1.38
24	p	311	CHL	CHD-C1D	4.61	1.47	1.38
24	3	311	CHL	CHD-C1D	4.60	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	313	CHL	CHD-C1D	4.60	1.47	1.38
24	N	317	CHL	CHC-C1C	4.60	1.47	1.38
24	7	310	CHL	CHC-C1C	4.60	1.47	1.38
24	y	312	CHL	C2C-C3C	4.60	1.46	1.36
24	S	605	CHL	CHD-C1D	4.60	1.47	1.38
24	G	318	CHL	CHD-C1D	4.60	1.47	1.38
24	1	310	CHL	CHD-C1D	4.60	1.47	1.38
24	Y	311	CHL	C2C-C3C	4.60	1.46	1.36
31	V	401	8CT	C06-C07	4.60	1.67	1.52
24	S	607	CHL	C2C-C3C	4.59	1.46	1.36
39	d	406	PL9	C3-C4	-4.59	1.42	1.49
31	C	615	8CT	C06-C07	4.59	1.66	1.52
24	G	309	CHL	CHC-C1C	4.59	1.47	1.38
24	Y	312	CHL	CHD-C1D	4.59	1.47	1.38
24	8	310	CHL	CHD-C1D	4.59	1.47	1.38
31	c	615	8CT	C06-C07	4.59	1.66	1.52
31	v	401	8CT	C06-C07	4.59	1.66	1.52
31	S	615	8CT	C06-C07	4.59	1.66	1.52
31	B	617	8CT	C06-C07	4.59	1.66	1.52
24	n	317	CHL	CHC-C1C	4.59	1.47	1.38
24	q	307	CHL	CHD-C1D	4.58	1.47	1.38
24	N	309	CHL	C2C-C3C	4.58	1.46	1.36
24	7	311	CHL	CHD-C1D	4.58	1.47	1.38
24	q	311	CHL	CHD-C1D	4.58	1.47	1.38
24	6	311	CHL	CHD-C1D	4.57	1.47	1.38
24	s	408	CHL	C2C-C3C	4.57	1.46	1.36
31	s	416	8CT	C06-C07	4.57	1.66	1.52
31	s	416	8CT	C19-C20	4.57	1.57	1.43
24	7	309	CHL	CHC-C1C	4.57	1.47	1.38
24	8	307	CHL	CHD-C1D	4.57	1.47	1.38
31	b	617	8CT	C06-C07	4.57	1.66	1.52
24	u	309	CHL	CHC-C1C	4.57	1.47	1.38
24	9	308	CHL	CHC-C1C	4.57	1.47	1.38
24	u	318	CHL	CHC-C1C	4.56	1.47	1.38
24	u	306	CHL	CHD-C1D	4.56	1.47	1.38
24	S	605	CHL	C2C-C3C	4.56	1.46	1.36
24	4	317	CHL	CHC-C1C	4.56	1.47	1.38
24	p	309	CHL	CHC-C1C	4.56	1.47	1.38
31	S	614	8CT	C06-C07	4.55	1.66	1.52
24	1	317	CHL	CHC-C1C	4.55	1.47	1.38
24	g	309	CHL	CHC-C1C	4.55	1.47	1.38
24	G	306	CHL	CHD-C1D	4.55	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	C2C-C3C	4.55	1.46	1.36
24	r	308	CHL	C2C-C3C	4.55	1.46	1.36
24	p	310	CHL	CHC-C1C	4.55	1.47	1.38
24	Y	319	CHL	C2C-C3C	4.54	1.46	1.36
24	y	311	CHL	C2C-C3C	4.54	1.46	1.36
24	q	309	CHL	C2C-C3C	4.54	1.46	1.36
24	2	306	CHL	C2C-C3C	4.54	1.46	1.36
24	s	406	CHL	C2C-C3C	4.54	1.46	1.36
24	2	310	CHL	C2C-C3C	4.53	1.46	1.36
24	R	605	CHL	C2C-C3C	4.53	1.46	1.36
31	S	614	8CT	C19-C20	4.53	1.57	1.43
31	D	410	8CT	C06-C07	4.53	1.66	1.52
31	s	415	8CT	C06-C07	4.53	1.66	1.52
24	y	313	CHL	C2C-C3C	4.53	1.46	1.36
24	R	608	CHL	CHD-C1D	4.53	1.47	1.38
24	5	310	CHL	C2C-C3C	4.53	1.46	1.36
24	5	306	CHL	C2C-C3C	4.53	1.46	1.36
24	n	309	CHL	C2C-C3C	4.53	1.46	1.36
24	N	311	CHL	CHD-C1D	4.53	1.47	1.38
24	g	306	CHL	CHD-C1D	4.53	1.47	1.38
31	S	615	8CT	C19-C20	4.53	1.57	1.43
24	r	303	CHL	C2C-C3C	4.52	1.46	1.36
24	6	310	CHL	O2A-CGA	4.52	1.45	1.30
24	S	607	CHL	CHD-C1D	4.51	1.47	1.38
24	Y	312	CHL	C2C-C3C	4.51	1.46	1.36
24	Y	319	CHL	CHD-C1D	4.51	1.47	1.38
24	2	310	CHL	CHD-C1D	4.51	1.47	1.38
24	3	310	CHL	O2A-CGA	4.51	1.45	1.30
24	u	310	CHL	CHC-C1C	4.51	1.47	1.38
24	6	308	CHL	CHC-C1C	4.51	1.47	1.38
31	s	415	8CT	C19-C20	4.50	1.57	1.43
24	S	601	CHL	C2C-C3C	4.50	1.46	1.36
24	s	408	CHL	CHD-C1D	4.50	1.47	1.38
24	n	305	CHL	CHD-C1D	4.50	1.47	1.38
24	s	402	CHL	C2C-C3C	4.50	1.46	1.36
24	4	304	CHL	CHC-C1C	4.50	1.47	1.38
24	r	302	CHL	O2A-CGA	4.50	1.45	1.30
24	S	607	CHL	O2A-CGA	4.50	1.45	1.30
31	d	410	8CT	C06-C07	4.50	1.66	1.52
24	5	310	CHL	CHD-C1D	4.49	1.47	1.38
24	1	309	CHL	CHC-C1C	4.49	1.47	1.38
24	2	312	CHL	CHD-C1D	4.49	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	305	CHL	CHD-C1D	4.49	1.47	1.38
24	Y	310	CHL	C2C-C3C	4.49	1.46	1.36
24	s	408	CHL	O2A-CGA	4.49	1.45	1.30
24	S	605	CHL	O2A-CGA	4.49	1.45	1.30
24	1	304	CHL	CHC-C1C	4.49	1.47	1.38
24	5	312	CHL	CHD-C1D	4.49	1.47	1.38
31	a	608	8CT	C06-C07	4.49	1.66	1.52
24	4	305	CHL	O2A-CGA	4.49	1.45	1.30
24	1	305	CHL	CHD-C1D	4.49	1.47	1.38
24	u	311	CHL	O2A-CGA	4.48	1.45	1.30
24	8	308	CHL	CHD-C1D	4.48	1.47	1.38
24	7	311	CHL	O2A-CGA	4.48	1.45	1.30
24	8	315	CHL	CHC-C1C	4.48	1.47	1.38
24	r	309	CHL	O2A-CGA	4.48	1.45	1.30
24	1	305	CHL	O2A-CGA	4.48	1.45	1.30
24	q	308	CHL	O2A-CGA	4.48	1.45	1.30
24	r	306	CHL	CHC-C1C	4.48	1.47	1.38
24	s	406	CHL	O2A-CGA	4.48	1.45	1.30
31	A	608	8CT	C06-C07	4.48	1.66	1.52
24	R	608	CHL	O2A-CGA	4.48	1.45	1.30
24	9	310	CHL	O2A-CGA	4.48	1.45	1.30
24	2	312	CHL	O2A-CGA	4.48	1.45	1.30
24	9	309	CHL	O2A-CGA	4.48	1.45	1.30
24	9	309	CHL	CHC-C1C	4.48	1.47	1.38
24	u	310	CHL	O2A-CGA	4.48	1.45	1.30
24	s	407	CHL	O2A-CGA	4.48	1.45	1.30
24	q	316	CHL	CHC-C1C	4.47	1.47	1.38
24	8	308	CHL	O2A-CGA	4.47	1.45	1.30
24	p	310	CHL	O2A-CGA	4.47	1.45	1.30
24	n	309	CHL	O2A-CGA	4.47	1.45	1.30
24	5	312	CHL	O2A-CGA	4.47	1.45	1.30
24	4	308	CHL	CHC-C1C	4.47	1.47	1.38
24	4	309	CHL	CHC-C1C	4.47	1.47	1.38
24	r	309	CHL	CHD-C1D	4.47	1.47	1.38
24	1	312	CHL	O2A-CGA	4.47	1.45	1.30
24	q	304	CHL	C2C-C3C	4.47	1.46	1.36
24	q	311	CHL	C2C-C3C	4.47	1.46	1.36
24	q	308	CHL	CHD-C1D	4.46	1.47	1.38
24	8	310	CHL	C2C-C3C	4.46	1.46	1.36
24	s	402	CHL	O2A-CGA	4.46	1.45	1.30
24	4	312	CHL	O2A-CGA	4.46	1.45	1.30
24	N	309	CHL	O2A-CGA	4.46	1.45	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	313	CHL	CHC-C1C	4.46	1.47	1.38
24	N	305	CHL	CHD-C1D	4.46	1.47	1.38
24	7	310	CHL	O2A-CGA	4.46	1.45	1.30
24	u	313	CHL	CHC-C1C	4.46	1.47	1.38
24	R	601	CHL	O2A-CGA	4.46	1.45	1.30
24	p	311	CHL	O2A-CGA	4.46	1.45	1.30
24	S	606	CHL	O2A-CGA	4.46	1.45	1.30
24	8	304	CHL	C2C-C3C	4.46	1.46	1.36
24	p	305	CHL	C2C-C3C	4.46	1.46	1.36
31	c	613	8CT	C06-C07	4.45	1.66	1.52
24	3	308	CHL	CHC-C1C	4.45	1.47	1.38
24	n	311	CHL	CHD-C1D	4.45	1.47	1.38
24	R	602	CHL	C2C-C3C	4.45	1.46	1.36
31	X	601	8CT	C06-C07	4.45	1.66	1.52
31	t	101	8CT	C06-C07	4.45	1.66	1.52
24	q	309	CHL	CHD-C1D	4.45	1.47	1.38
24	9	312	CHL	CHC-C1C	4.44	1.47	1.38
31	x	601	8CT	C06-C07	4.44	1.66	1.52
24	G	310	CHL	CHC-C1C	4.44	1.47	1.38
24	1	308	CHL	CHC-C1C	4.44	1.47	1.38
31	C	613	8CT	C06-C07	4.44	1.66	1.52
24	7	305	CHL	C2C-C3C	4.44	1.46	1.36
24	S	601	CHL	O2A-CGA	4.44	1.45	1.30
24	5	309	CHL	CHC-C1C	4.44	1.47	1.38
31	T	101	8CT	C06-C07	4.44	1.66	1.52
24	8	304	CHL	CHD-C1D	4.43	1.47	1.38
24	9	310	CHL	CHC-C1C	4.43	1.47	1.38
24	u	311	CHL	CHC-C1C	4.43	1.47	1.38
24	Y	311	CHL	CHD-C1D	4.43	1.47	1.38
24	p	306	CHL	C2C-C3C	4.43	1.46	1.36
24	y	311	CHL	CHD-C1D	4.43	1.47	1.38
24	q	310	CHL	C2C-C3C	4.43	1.46	1.36
24	y	312	CHL	CHD-C1D	4.43	1.47	1.38
24	8	309	CHL	C2C-C3C	4.42	1.46	1.36
24	r	308	CHL	CHD-C1D	4.42	1.47	1.38
24	q	308	CHL	C2C-C3C	4.42	1.46	1.36
24	g	310	CHL	CHC-C1C	4.42	1.47	1.38
24	R	605	CHL	CHD-C1D	4.42	1.47	1.38
24	n	308	CHL	CHC-C1C	4.42	1.47	1.38
24	2	306	CHL	CHD-C1D	4.41	1.47	1.38
24	n	310	CHL	CHC-C1C	4.41	1.47	1.38
24	r	307	CHL	CHD-C1D	4.41	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	304	CHL	CHD-C1D	4.41	1.47	1.38
24	7	306	CHL	C2C-C3C	4.41	1.46	1.36
24	6	310	CHL	CHC-C1C	4.41	1.47	1.38
31	c	615	8CT	C19-C20	4.40	1.57	1.43
24	3	317	CHL	CHC-C1C	4.40	1.47	1.38
24	5	306	CHL	CHD-C1D	4.40	1.46	1.38
24	p	305	CHL	CHD-C1D	4.40	1.46	1.38
24	u	306	CHL	CHC-C1C	4.40	1.47	1.38
31	b	617	8CT	C19-C20	4.39	1.57	1.43
24	5	311	CHL	CHC-C1C	4.39	1.47	1.38
24	n	309	CHL	CHD-C1D	4.39	1.46	1.38
24	3	310	CHL	CHC-C1C	4.39	1.47	1.38
24	N	309	CHL	CHD-C1D	4.39	1.46	1.38
24	n	304	CHL	CHC-C1C	4.39	1.47	1.38
24	N	310	CHL	CHC-C1C	4.39	1.47	1.38
24	R	601	CHL	CHC-C1C	4.39	1.47	1.38
24	u	305	CHL	CHC-C1C	4.38	1.47	1.38
24	S	613	CHL	C2C-C3C	4.38	1.46	1.36
24	R	607	CHL	CHD-C1D	4.38	1.46	1.38
24	2	318	CHL	CHC-C1C	4.38	1.47	1.38
24	r	302	CHL	CHC-C1C	4.38	1.47	1.38
24	5	318	CHL	CHC-C1C	4.38	1.47	1.38
24	n	305	CHL	CHC-C1C	4.38	1.47	1.38
24	8	308	CHL	C2C-C3C	4.38	1.46	1.36
24	Y	310	CHL	CHD-C1D	4.38	1.46	1.38
31	v	401	8CT	C19-C20	4.38	1.57	1.43
24	R	605	CHL	C3A-C2A	-4.38	1.50	1.54
24	s	414	CHL	C2C-C3C	4.38	1.46	1.36
24	2	309	CHL	CHC-C1C	4.37	1.47	1.38
24	G	313	CHL	CHC-C1C	4.37	1.47	1.38
24	u	312	CHL	CHC-C1C	4.37	1.47	1.38
24	6	312	CHL	CHC-C1C	4.37	1.47	1.38
24	8	309	CHL	CHD-C1D	4.37	1.46	1.38
31	C	615	8CT	C19-C20	4.37	1.57	1.43
24	R	606	CHL	CHD-C1D	4.37	1.46	1.38
31	T	101	8CT	C19-C20	4.37	1.57	1.43
24	3	309	CHL	O2A-CGA	4.36	1.46	1.33
24	g	311	CHL	CHC-C1C	4.36	1.47	1.38
31	c	614	8CT	C06-C07	4.36	1.66	1.52
24	G	311	CHL	CHC-C1C	4.36	1.47	1.38
24	6	317	CHL	CHC-C1C	4.36	1.47	1.38
24	3	312	CHL	CHC-C1C	4.36	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	305	CHL	CHC-C1C	4.36	1.47	1.38
24	p	312	CHL	C2C-C3C	4.36	1.46	1.36
24	S	601	CHL	CHD-C1D	4.36	1.46	1.38
24	q	310	CHL	CHD-C1D	4.36	1.46	1.38
31	B	617	8CT	C19-C20	4.36	1.56	1.43
31	C	614	8CT	C06-C07	4.35	1.66	1.52
24	S	613	CHL	CHD-C1D	4.35	1.46	1.38
24	N	304	CHL	CHC-C1C	4.35	1.47	1.38
24	6	305	CHL	CHC-C1C	4.35	1.47	1.38
24	Y	309	CHL	C2C-C3C	4.35	1.46	1.36
24	N	311	CHL	O2A-CGA	4.35	1.46	1.33
31	t	101	8CT	C19-C20	4.35	1.56	1.43
24	q	307	CHL	CHC-C1C	4.34	1.47	1.38
24	R	602	CHL	CHD-C1D	4.34	1.46	1.38
24	r	303	CHL	CHD-C1D	4.34	1.46	1.38
24	G	312	CHL	CHC-C1C	4.34	1.47	1.38
24	n	311	CHL	O2A-CGA	4.34	1.46	1.33
24	N	312	CHL	O2A-CGA	4.34	1.46	1.33
24	N	308	CHL	CHC-C1C	4.34	1.47	1.38
24	y	318	CHL	C2C-C3C	4.34	1.46	1.36
31	V	401	8CT	C19-C20	4.33	1.56	1.43
24	Y	317	CHL	C2C-C3C	4.33	1.46	1.36
24	6	304	CHL	O2A-CGA	4.33	1.46	1.33
24	6	309	CHL	O2A-CGA	4.33	1.46	1.33
24	y	318	CHL	CHD-C1D	4.33	1.46	1.38
24	G	313	CHL	O2A-CGA	4.33	1.46	1.33
24	s	414	CHL	CHD-C1D	4.33	1.46	1.38
24	3	309	CHL	CHC-C1C	4.33	1.47	1.38
24	y	310	CHL	C2C-C3C	4.33	1.46	1.36
24	9	305	CHL	O2A-CGA	4.33	1.46	1.33
24	n	310	CHL	O2A-CGA	4.32	1.46	1.33
24	7	305	CHL	CHD-C1D	4.32	1.46	1.38
31	A	608	8CT	C19-C20	4.32	1.56	1.43
24	9	311	CHL	CHC-C1C	4.32	1.47	1.38
24	4	312	CHL	CHC-C1C	4.32	1.47	1.38
24	1	312	CHL	CHC-C1C	4.32	1.47	1.38
31	c	613	8CT	C19-C20	4.32	1.56	1.43
24	3	305	CHL	CHC-C1C	4.32	1.47	1.38
24	3	304	CHL	O2A-CGA	4.32	1.46	1.33
24	u	306	CHL	O2A-CGA	4.31	1.45	1.33
24	2	311	CHL	CHC-C1C	4.31	1.47	1.38
24	s	402	CHL	CHD-C1D	4.31	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	303	CHL	CHC-C1C	4.31	1.47	1.38
31	X	601	8CT	C19-C20	4.31	1.56	1.43
24	7	312	CHL	C2C-C3C	4.31	1.46	1.36
31	a	608	8CT	C19-C20	4.31	1.56	1.43
31	d	410	8CT	C19-C20	4.31	1.56	1.43
31	D	410	8CT	C19-C20	4.31	1.56	1.43
37	C	619	DGD	O1G-C1A	4.31	1.45	1.33
24	s	403	CHL	C2C-C3C	4.31	1.46	1.36
24	N	310	CHL	O2A-CGA	4.31	1.45	1.33
24	n	312	CHL	O2A-CGA	4.31	1.45	1.33
24	g	313	CHL	O2A-CGA	4.31	1.45	1.33
24	6	305	CHL	O2A-CGA	4.30	1.45	1.33
24	3	305	CHL	O2A-CGA	4.30	1.45	1.33
24	S	602	CHL	C2C-C3C	4.30	1.46	1.36
24	G	306	CHL	O2A-CGA	4.30	1.45	1.33
24	5	310	CHL	C3A-C2A	-4.30	1.50	1.54
37	c	618	DGD	O1G-C1A	4.30	1.45	1.33
24	R	607	CHL	O2A-CGA	4.29	1.45	1.33
24	Y	317	CHL	CHD-C1D	4.29	1.46	1.38
24	g	306	CHL	O2A-CGA	4.29	1.45	1.33
24	Y	319	CHL	O2A-CGA	4.29	1.45	1.33
24	q	309	CHL	O2A-CGA	4.29	1.45	1.33
24	G	311	CHL	O2A-CGA	4.29	1.45	1.33
31	c	614	8CT	C19-C20	4.29	1.56	1.43
24	8	307	CHL	CHC-C1C	4.29	1.47	1.38
24	q	303	CHL	O2A-CGA	4.29	1.45	1.33
24	p	311	CHL	CHC-C1C	4.28	1.47	1.38
31	C	613	8CT	C19-C20	4.28	1.56	1.43
24	8	304	CHL	O2A-CGA	4.28	1.45	1.33
24	N	305	CHL	O2A-CGA	4.28	1.45	1.33
24	q	304	CHL	O2A-CGA	4.28	1.45	1.33
24	r	308	CHL	O2A-CGA	4.28	1.45	1.33
24	g	311	CHL	O2A-CGA	4.28	1.45	1.33
24	p	305	CHL	O2A-CGA	4.28	1.45	1.33
24	y	313	CHL	O2A-CGA	4.28	1.45	1.33
24	9	305	CHL	CHC-C1C	4.28	1.47	1.38
24	8	303	CHL	O2A-CGA	4.27	1.45	1.33
24	8	309	CHL	O2A-CGA	4.27	1.45	1.33
24	y	311	CHL	O2A-CGA	4.27	1.45	1.33
24	q	303	CHL	CHC-C1C	4.27	1.47	1.38
24	R	606	CHL	O2A-CGA	4.27	1.45	1.33
24	n	305	CHL	O2A-CGA	4.27	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	304	CHL	CHC-C1C	4.27	1.47	1.38
26	9	303	0IE	C15-C16	4.27	1.41	1.35
33	d	411	LMG	O8-C28	4.27	1.45	1.33
33	D	411	LMG	O8-C28	4.27	1.45	1.33
31	x	601	8CT	C19-C20	4.27	1.56	1.43
24	p	318	CHL	CHC-C1C	4.27	1.47	1.38
24	G	312	CHL	O2A-CGA	4.26	1.45	1.33
24	u	305	CHL	O2A-CGA	4.26	1.45	1.33
24	7	305	CHL	O2A-CGA	4.26	1.45	1.33
24	3	311	CHL	CHC-C1C	4.26	1.47	1.38
24	Y	311	CHL	O2A-CGA	4.26	1.45	1.33
24	7	311	CHL	CHC-C1C	4.26	1.47	1.38
24	Y	312	CHL	O2A-CGA	4.26	1.45	1.33
24	y	305	CHL	C2C-C3C	4.26	1.45	1.36
24	q	310	CHL	O2A-CGA	4.26	1.45	1.33
24	4	310	CHL	CHC-C1C	4.26	1.47	1.38
24	6	309	CHL	CHC-C1C	4.26	1.47	1.38
24	s	402	CHL	CHC-C1C	4.26	1.47	1.38
24	S	602	CHL	O2A-CGA	4.25	1.45	1.33
24	6	304	CHL	CHC-C1C	4.25	1.47	1.38
24	r	307	CHL	O2A-CGA	4.25	1.45	1.33
24	8	310	CHL	O2A-CGA	4.25	1.45	1.33
24	1	310	CHL	CHC-C1C	4.25	1.47	1.38
24	q	311	CHL	O2A-CGA	4.25	1.45	1.33
24	Y	304	CHL	CHD-C1D	4.25	1.46	1.38
24	s	403	CHL	O2A-CGA	4.25	1.45	1.33
24	y	312	CHL	O2A-CGA	4.25	1.45	1.33
24	y	310	CHL	CHD-C1D	4.25	1.46	1.38
24	9	304	CHL	O2A-CGA	4.24	1.45	1.33
24	y	305	CHL	CHD-C1D	4.24	1.46	1.38
24	g	312	CHL	O2A-CGA	4.24	1.45	1.33
24	Y	310	CHL	O2A-CGA	4.24	1.45	1.33
24	5	313	CHL	CHC-C1C	4.24	1.47	1.38
24	G	318	CHL	C3A-C2A	-4.24	1.50	1.54
26	u	303	0IE	C15-C16	4.24	1.41	1.35
24	g	305	CHL	CHC-C1C	4.24	1.47	1.38
24	g	305	CHL	O2A-CGA	4.24	1.45	1.33
24	2	306	CHL	CHC-C1C	4.24	1.47	1.38
31	C	614	8CT	C19-C20	4.24	1.56	1.43
24	7	318	CHL	CHC-C1C	4.24	1.47	1.38
24	2	310	CHL	CHC-C1C	4.23	1.47	1.38
24	n	304	CHL	O2A-CGA	4.23	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	306	CHL	O2A-CGA	4.23	1.45	1.33
24	N	304	CHL	O2A-CGA	4.23	1.45	1.33
24	7	306	CHL	O2A-CGA	4.23	1.45	1.33
24	g	318	CHL	C3A-C2A	-4.23	1.50	1.54
24	Y	304	CHL	C2C-C3C	4.23	1.45	1.36
24	Y	309	CHL	CHD-C1D	4.23	1.46	1.38
24	y	306	CHL	CHD-C1D	4.22	1.46	1.38
24	g	318	CHL	CHC-C1C	4.22	1.47	1.38
24	g	312	CHL	CHC-C1C	4.21	1.47	1.38
24	2	313	CHL	CHC-C1C	4.21	1.47	1.38
24	Y	305	CHL	C2C-C3C	4.21	1.45	1.36
24	G	305	CHL	CHC-C1C	4.21	1.47	1.38
24	G	318	CHL	CHC-C1C	4.21	1.47	1.38
24	Y	305	CHL	CHD-C1D	4.21	1.46	1.38
24	G	305	CHL	O2A-CGA	4.20	1.45	1.33
24	6	311	CHL	CHC-C1C	4.20	1.47	1.38
24	y	306	CHL	C2C-C3C	4.20	1.45	1.36
31	S	615	8CT	C24-C25	4.20	1.56	1.43
24	3	304	CHL	CHC-C1C	4.20	1.47	1.38
33	B	619	LMG	O8-C28	4.20	1.45	1.33
24	5	306	CHL	CHC-C1C	4.20	1.47	1.38
24	p	312	CHL	CHD-C1D	4.20	1.46	1.38
24	2	310	CHL	C3A-C2A	-4.20	1.50	1.54
24	N	312	CHL	CHC-C1C	4.19	1.47	1.38
33	m	101	LMG	O8-C28	4.18	1.45	1.33
31	s	416	8CT	C24-C25	4.18	1.56	1.43
24	7	312	CHL	CHD-C1D	4.18	1.46	1.38
24	N	311	CHL	CHC-C1C	4.18	1.47	1.38
24	8	308	CHL	CHC-C1C	4.18	1.47	1.38
24	5	310	CHL	CHC-C1C	4.18	1.47	1.38
31	s	415	8CT	C11-C12	4.17	1.54	1.45
24	S	601	CHL	CHC-C1C	4.17	1.47	1.38
24	s	406	CHL	CHC-C1C	4.17	1.47	1.38
24	S	605	CHL	CHC-C1C	4.17	1.47	1.38
24	R	605	CHL	CHC-C1C	4.17	1.47	1.38
24	n	312	CHL	CHC-C1C	4.17	1.47	1.38
24	G	306	CHL	CHC-C1C	4.16	1.47	1.38
24	4	305	CHL	CHC-C1C	4.16	1.47	1.38
24	p	313	CHL	CHC-C1C	4.15	1.47	1.38
24	q	308	CHL	CHC-C1C	4.15	1.46	1.38
24	y	309	CHL	CHC-C1C	4.15	1.46	1.38
31	S	614	8CT	C11-C12	4.14	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	305	CHL	CHC-C1C	4.14	1.46	1.38
24	s	408	CHL	CHC-C1C	4.14	1.46	1.38
26	u	303	0IE	C11-C12	4.14	1.41	1.35
31	S	615	8CT	C14-C13	4.14	1.56	1.43
24	y	306	CHL	CHC-C1C	4.14	1.46	1.38
24	1	305	CHL	CHC-C1C	4.14	1.46	1.38
24	7	306	CHL	CHD-C1D	4.14	1.46	1.38
26	9	303	0IE	C11-C12	4.14	1.41	1.35
24	q	309	CHL	CHC-C1C	4.14	1.46	1.38
24	Y	319	CHL	CHC-C1C	4.13	1.46	1.38
26	u	302	0IE	C8-C7	4.13	1.41	1.35
24	s	403	CHL	CHC-C1C	4.13	1.46	1.38
31	s	416	8CT	C14-C13	4.13	1.56	1.43
24	n	311	CHL	CHC-C1C	4.13	1.46	1.38
33	D	401	LMG	O8-C28	4.13	1.45	1.33
26	u	303	0IE	C8-C7	4.13	1.41	1.35
24	r	307	CHL	CHC-C1C	4.13	1.46	1.38
33	C	618	LMG	O8-C28	4.12	1.45	1.33
24	R	606	CHL	CHC-C1C	4.12	1.46	1.38
24	2	305	CHL	CHC-C1C	4.12	1.46	1.38
24	Y	305	CHL	CHC-C1C	4.12	1.46	1.38
24	S	606	CHL	CHC-C1C	4.12	1.46	1.38
24	p	306	CHL	CHD-C1D	4.12	1.46	1.38
24	s	407	CHL	CHC-C1C	4.12	1.46	1.38
24	Y	308	CHL	CHC-C1C	4.11	1.46	1.38
24	7	313	CHL	CHC-C1C	4.11	1.46	1.38
24	R	608	CHL	CHC-C1C	4.11	1.46	1.38
24	g	306	CHL	CHC-C1C	4.11	1.46	1.38
24	8	304	CHL	CHC-C1C	4.11	1.46	1.38
24	y	306	CHL	O2A-CGA	4.10	1.45	1.33
24	s	403	CHL	CHD-C1D	4.10	1.46	1.38
31	S	614	8CT	C24-C25	4.10	1.56	1.43
24	q	304	CHL	CHC-C1C	4.10	1.46	1.38
24	r	303	CHL	CHC-C1C	4.10	1.46	1.38
31	v	401	8CT	C24-C25	4.10	1.56	1.43
24	R	602	CHL	CHC-C1C	4.10	1.46	1.38
33	d	401	LMG	O8-C28	4.10	1.45	1.33
24	y	313	CHL	CHC-C1C	4.10	1.46	1.38
31	V	401	8CT	C24-C25	4.10	1.56	1.43
24	Y	312	CHL	CHC-C1C	4.09	1.46	1.38
31	s	415	8CT	C24-C25	4.09	1.56	1.43
24	S	602	CHL	CHD-C1D	4.09	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	302	0IE	C11-C12	4.09	1.41	1.35
24	Y	304	CHL	O2A-CGA	4.09	1.45	1.33
24	S	613	CHL	CHC-C1C	4.09	1.46	1.38
24	r	309	CHL	CHC-C1C	4.09	1.46	1.38
24	S	602	CHL	CHC-C1C	4.08	1.46	1.38
24	y	305	CHL	O2A-CGA	4.08	1.45	1.33
24	2	312	CHL	CHC-C1C	4.08	1.46	1.38
26	3	303	0IE	C15-C16	4.08	1.41	1.35
24	s	414	CHL	CHC-C1C	4.08	1.46	1.38
26	9	302	0IE	C8-C7	4.07	1.41	1.35
24	7	306	CHL	CHC-C1C	4.07	1.46	1.38
24	Y	305	CHL	O2A-CGA	4.07	1.45	1.33
33	i	101	LMG	O8-C28	4.06	1.45	1.33
26	u	302	0IE	C11-C12	4.06	1.41	1.35
26	9	302	0IE	C11-C12	4.06	1.41	1.35
26	3	303	0IE	C11-C12	4.05	1.41	1.35
24	Y	309	CHL	O2A-CGA	4.05	1.45	1.33
24	u	312	CHL	O2A-CGA	4.05	1.45	1.33
26	3	303	0IE	C8-C7	4.05	1.41	1.35
24	p	312	CHL	O2A-CGA	4.05	1.45	1.33
26	n	302	0IE	C11-C12	4.05	1.41	1.35
24	Y	309	CHL	CHC-C1C	4.05	1.46	1.38
24	R	602	CHL	O2A-CGA	4.04	1.45	1.33
26	1	302	0IE	C11-C12	4.04	1.41	1.35
24	y	310	CHL	O2A-CGA	4.04	1.45	1.33
24	r	303	CHL	O2A-CGA	4.04	1.45	1.33
24	G	310	CHL	O2A-CGA	4.04	1.45	1.33
26	p	302	0IE	C11-C12	4.04	1.41	1.35
31	D	410	8CT	C24-C25	4.04	1.56	1.43
24	9	311	CHL	O2A-CGA	4.04	1.45	1.33
24	2	311	CHL	O2A-CGA	4.03	1.45	1.33
24	5	311	CHL	O2A-CGA	4.03	1.45	1.33
24	1	311	CHL	CHC-C1C	4.03	1.46	1.38
24	p	306	CHL	CHC-C1C	4.03	1.46	1.38
24	g	310	CHL	O2A-CGA	4.03	1.45	1.33
31	t	101	8CT	C24-C25	4.03	1.55	1.43
31	d	410	8CT	C24-C25	4.03	1.55	1.43
24	y	310	CHL	CHC-C1C	4.03	1.46	1.38
24	y	311	CHL	CHC-C1C	4.03	1.46	1.38
26	6	302	0IE	C8-C7	4.03	1.41	1.35
24	s	409	CHL	O2A-CGA	4.03	1.45	1.33
24	5	312	CHL	CHC-C1C	4.02	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	T	101	8CT	C24-C25	4.02	1.55	1.43
24	S	608	CHL	O2A-CGA	4.02	1.45	1.33
24	9	309	CHL	CHC-C4B	4.02	1.48	1.39
24	4	311	CHL	CHC-C1C	4.02	1.46	1.38
26	7	302	0IE	C11-C12	4.02	1.41	1.35
24	7	312	CHL	O2A-CGA	4.02	1.45	1.33
24	S	607	CHL	CHC-C1C	4.02	1.46	1.38
26	3	302	0IE	C8-C7	4.02	1.41	1.35
26	9	303	0IE	C8-C7	4.01	1.41	1.35
24	n	317	CHL	CHC-C4B	4.01	1.48	1.39
24	s	409	CHL	CHC-C1C	4.01	1.46	1.38
24	p	310	CHL	CHC-C4B	4.01	1.48	1.39
26	r	315	0IE	C8-C7	4.01	1.41	1.35
24	2	306	CHL	O2A-CGA	4.01	1.45	1.33
24	N	317	CHL	CHC-C4B	4.01	1.48	1.39
26	N	302	0IE	C11-C12	4.01	1.41	1.35
26	1	302	0IE	C8-C7	4.01	1.41	1.35
26	2	303	0IE	C11-C12	4.00	1.41	1.35
24	3	317	CHL	C3A-C2A	-4.00	1.50	1.54
31	b	617	8CT	C24-C25	4.00	1.55	1.43
24	u	310	CHL	CHC-C4B	4.00	1.48	1.39
26	4	302	0IE	C15-C16	3.99	1.41	1.35
26	n	302	0IE	C15-C16	3.99	1.41	1.35
31	c	615	8CT	C24-C25	3.99	1.55	1.43
24	g	309	CHL	CHC-C4B	3.99	1.48	1.39
24	Y	317	CHL	CHC-C1C	3.99	1.46	1.38
31	C	613	8CT	C24-C25	3.99	1.55	1.43
24	5	306	CHL	O2A-CGA	3.99	1.45	1.33
37	C	620	DGD	O1G-C1A	3.99	1.45	1.33
24	Y	310	CHL	CHC-C1C	3.98	1.46	1.38
26	R	614	0IE	C8-C7	3.98	1.41	1.35
26	5	303	0IE	C11-C12	3.98	1.41	1.35
26	9	302	0IE	C15-C16	3.98	1.41	1.35
26	p	302	0IE	C8-C7	3.98	1.41	1.35
31	X	601	8CT	C24-C25	3.98	1.55	1.43
24	7	310	CHL	CHC-C4B	3.98	1.48	1.39
26	R	614	0IE	C11-C12	3.98	1.41	1.35
31	s	416	8CT	C11-C12	3.98	1.54	1.45
26	G	302	0IE	C11-C12	3.97	1.41	1.35
31	B	617	8CT	C24-C25	3.97	1.55	1.43
26	4	302	0IE	C8-C7	3.97	1.41	1.35
31	c	613	8CT	C24-C25	3.97	1.55	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	308	CHL	CHC-C4B	3.97	1.48	1.39
24	1	308	CHL	CHC-C4B	3.97	1.48	1.39
24	4	317	CHL	CHC-C4B	3.97	1.48	1.39
26	7	302	0IE	C8-C7	3.96	1.41	1.35
24	7	309	CHL	CHD-C4C	3.96	1.48	1.39
31	C	615	8CT	C24-C25	3.96	1.55	1.43
31	x	601	8CT	C24-C25	3.96	1.55	1.43
24	y	318	CHL	CHC-C1C	3.96	1.46	1.38
24	1	317	CHL	CHC-C4B	3.96	1.48	1.39
26	n	302	0IE	C8-C7	3.96	1.41	1.35
24	p	309	CHL	CHD-C4C	3.96	1.48	1.39
24	8	310	CHL	CHC-C1C	3.96	1.46	1.38
26	g	302	0IE	C11-C12	3.95	1.41	1.35
24	9	317	CHL	CHC-C4B	3.95	1.48	1.39
24	u	309	CHL	CHC-C4B	3.95	1.48	1.39
24	N	317	CHL	CHD-C4C	3.95	1.48	1.39
24	u	318	CHL	CHC-C4B	3.95	1.48	1.39
24	S	608	CHL	CHC-C1C	3.95	1.46	1.38
24	q	311	CHL	CHC-C1C	3.95	1.46	1.38
24	G	309	CHL	CHC-C4B	3.95	1.48	1.39
26	1	302	0IE	C15-C16	3.94	1.41	1.35
24	Y	311	CHL	CHC-C1C	3.94	1.46	1.38
26	N	302	0IE	C15-C16	3.94	1.41	1.35
24	N	309	CHL	CHC-C1C	3.94	1.46	1.38
24	6	317	CHL	C3A-C2A	-3.94	1.50	1.54
24	7	318	CHL	C3A-C2A	-3.94	1.50	1.54
24	4	309	CHL	CHC-C4B	3.94	1.48	1.39
24	4	308	CHL	CHC-C4B	3.94	1.48	1.39
24	u	318	CHL	CHD-C4C	3.94	1.48	1.39
31	S	615	8CT	C11-C12	3.94	1.54	1.45
26	6	302	0IE	C11-C12	3.94	1.41	1.35
24	4	304	CHL	CHC-C4B	3.93	1.48	1.39
24	G	309	CHL	CHD-C4C	3.93	1.48	1.39
24	9	317	CHL	CHD-C4C	3.93	1.48	1.39
24	9	308	CHL	CHD-C4C	3.93	1.48	1.39
26	G	302	0IE	C8-C7	3.93	1.41	1.35
24	1	309	CHL	CHC-C4B	3.92	1.48	1.39
24	r	308	CHL	CHC-C1C	3.92	1.46	1.38
24	u	306	CHL	CHC-C4B	3.92	1.48	1.39
26	5	303	0IE	C15-C16	3.92	1.41	1.35
26	g	302	0IE	C8-C7	3.92	1.41	1.35
24	p	318	CHL	C3A-C2A	-3.92	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	302	0IE	C15-C16	3.92	1.41	1.35
24	1	304	CHL	CHD-C4C	3.91	1.48	1.39
37	c	619	DGD	O1G-C1A	3.91	1.44	1.33
24	n	317	CHL	CHD-C4C	3.91	1.48	1.39
26	3	302	0IE	C11-C12	3.91	1.41	1.35
24	n	309	CHL	CHC-C1C	3.91	1.46	1.38
24	R	607	CHL	CHC-C1C	3.91	1.46	1.38
24	1	317	CHL	CHD-C4C	3.91	1.48	1.39
24	y	312	CHL	CHC-C1C	3.91	1.46	1.38
26	r	315	0IE	C11-C12	3.91	1.41	1.35
26	5	303	0IE	C8-C7	3.90	1.41	1.35
25	4	316	CLA	C1D-ND	3.90	1.42	1.37
24	p	312	CHL	CHC-C1C	3.90	1.46	1.38
24	g	313	CHL	CHD-C4C	3.90	1.48	1.39
24	6	308	CHL	CHD-C4C	3.90	1.48	1.39
24	8	315	CHL	CHC-C4B	3.90	1.48	1.39
24	g	309	CHL	CHD-C4C	3.90	1.48	1.39
31	a	608	8CT	C24-C25	3.90	1.55	1.43
24	9	310	CHL	CHC-C4B	3.89	1.48	1.39
31	c	614	8CT	C24-C25	3.89	1.55	1.43
24	u	309	CHL	CHD-C4C	3.89	1.48	1.39
24	3	308	CHL	CHC-C4B	3.89	1.48	1.39
33	w	201	LMG	O8-C28	3.89	1.44	1.33
31	C	614	8CT	C24-C25	3.88	1.55	1.43
24	4	317	CHL	CHD-C4C	3.88	1.48	1.39
24	3	312	CHL	CHD-C4C	3.88	1.48	1.39
24	u	311	CHL	CHC-C4B	3.88	1.48	1.39
24	q	316	CHL	CHC-C4B	3.88	1.48	1.39
24	N	305	CHL	CHC-C4B	3.87	1.48	1.39
24	5	309	CHL	CHC-C4B	3.87	1.48	1.39
31	A	608	8CT	C24-C25	3.87	1.55	1.43
39	D	406	PL9	C6-C1	-3.87	1.41	1.48
24	6	312	CHL	CHD-C4C	3.87	1.48	1.39
26	p	302	0IE	C15-C16	3.87	1.40	1.35
24	p	309	CHL	CHC-C4B	3.87	1.48	1.39
24	u	313	CHL	CHD-C4C	3.87	1.48	1.39
24	1	308	CHL	CHD-C4C	3.87	1.48	1.39
24	3	308	CHL	CHD-C4C	3.87	1.48	1.39
24	G	313	CHL	CHD-C4C	3.86	1.48	1.39
25	N	316	CLA	C1D-ND	3.86	1.42	1.37
24	3	305	CHL	CHC-C4B	3.86	1.48	1.39
24	7	312	CHL	CHC-C1C	3.86	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	308	CHL	CHC-C4B	3.86	1.48	1.39
31	s	415	8CT	C14-C13	3.86	1.55	1.43
26	g	302	0IE	C15-C16	3.86	1.40	1.35
24	6	305	CHL	CHC-C4B	3.86	1.48	1.39
24	u	313	CHL	CHC-C4B	3.86	1.48	1.39
39	d	406	PL9	C6-C1	-3.86	1.41	1.48
24	4	308	CHL	CHD-C4C	3.86	1.48	1.39
31	S	614	8CT	C14-C13	3.86	1.55	1.43
26	2	303	0IE	C15-C16	3.86	1.40	1.35
24	1	304	CHL	CHC-C4B	3.86	1.48	1.39
26	7	302	0IE	C15-C16	3.86	1.40	1.35
24	s	403	CHL	C1D-ND	-3.86	1.33	1.37
33	w	201	LMG	O7-C10	3.86	1.45	1.34
24	p	305	CHL	CHC-C1C	3.86	1.46	1.38
24	G	310	CHL	CHD-C4C	3.85	1.48	1.39
24	4	304	CHL	CHD-C4C	3.85	1.48	1.39
24	q	310	CHL	CHC-C1C	3.85	1.46	1.38
26	G	302	0IE	C15-C16	3.85	1.40	1.35
24	7	309	CHL	CHC-C4B	3.85	1.48	1.39
24	1	309	CHL	CHD-C4C	3.85	1.48	1.39
31	S	615	8CT	C28-C29	3.85	1.41	1.32
24	n	304	CHL	CHC-C4B	3.84	1.48	1.39
24	S	602	CHL	C1D-ND	-3.84	1.33	1.37
26	6	302	0IE	C15-C16	3.84	1.40	1.35
24	5	318	CHL	CHC-C4B	3.84	1.48	1.39
24	g	313	CHL	CHC-C4B	3.84	1.48	1.39
24	2	309	CHL	CHC-C4B	3.84	1.48	1.39
24	n	305	CHL	CHC-C4B	3.84	1.48	1.39
26	N	302	0IE	C8-C7	3.84	1.40	1.35
24	6	310	CHL	CHC-C4B	3.84	1.48	1.39
24	n	304	CHL	CHD-C4C	3.84	1.48	1.39
25	4	315	CLA	C1D-ND	3.84	1.42	1.37
24	r	302	CHL	CHC-C4B	3.84	1.48	1.39
24	8	309	CHL	CHC-C1C	3.84	1.46	1.38
24	g	310	CHL	CHC-C4B	3.84	1.48	1.39
24	G	310	CHL	CHC-C4B	3.84	1.48	1.39
26	2	303	0IE	C8-C7	3.84	1.40	1.35
24	R	601	CHL	CHC-C4B	3.84	1.48	1.39
24	6	312	CHL	CHC-C4B	3.84	1.48	1.39
24	6	317	CHL	CHC-C4B	3.84	1.48	1.39
24	3	317	CHL	CHC-C4B	3.83	1.48	1.39
24	8	315	CHL	CHD-C4C	3.83	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	312	CHL	CHD-C4C	3.83	1.48	1.39
24	N	304	CHL	CHD-C4C	3.83	1.48	1.39
26	g	303	0IE	C11-C12	3.83	1.40	1.35
25	u	314	CLA	C1D-ND	3.83	1.42	1.37
24	g	310	CHL	CHD-C4C	3.82	1.48	1.39
24	9	312	CHL	CHC-C4B	3.82	1.48	1.39
24	u	305	CHL	CHD-C4C	3.82	1.48	1.39
24	4	309	CHL	CHD-C4C	3.82	1.48	1.39
31	s	416	8CT	C28-C29	3.82	1.41	1.32
26	r	315	0IE	C15-C16	3.82	1.40	1.35
24	6	310	CHL	CHD-C4C	3.82	1.48	1.39
24	N	304	CHL	CHC-C4B	3.82	1.48	1.39
24	u	312	CHL	CHC-C4B	3.82	1.48	1.39
30	d	408	LHG	O8-C23	3.82	1.44	1.33
24	n	308	CHL	CHC-C4B	3.82	1.48	1.39
24	n	310	CHL	CHC-C4B	3.82	1.48	1.39
26	p	303	0IE	C15-C16	3.82	1.40	1.35
31	c	615	8CT	C14-C13	3.82	1.55	1.43
24	3	312	CHL	CHC-C4B	3.81	1.48	1.39
24	2	311	CHL	CHC-C4B	3.81	1.48	1.39
25	R	613	CLA	C1D-ND	3.81	1.42	1.37
24	1	317	CHL	OBD-CAD	3.81	1.29	1.22
25	a	610	CLA	C1D-ND	3.81	1.42	1.37
24	2	318	CHL	CHC-C4B	3.81	1.47	1.39
24	7	305	CHL	CHC-C1C	3.81	1.46	1.38
24	4	310	CHL	CHC-C4B	3.81	1.47	1.39
24	3	310	CHL	CHC-C4B	3.81	1.47	1.39
24	u	310	CHL	CHD-C4C	3.81	1.47	1.39
25	r	314	CLA	C1D-ND	3.81	1.42	1.37
24	7	311	CHL	CHC-C4B	3.80	1.47	1.39
31	s	415	8CT	C28-C29	3.80	1.41	1.32
24	9	311	CHL	CHC-C4B	3.80	1.47	1.39
24	6	309	CHL	CHC-C4B	3.80	1.47	1.39
24	N	310	CHL	CHC-C4B	3.80	1.47	1.39
31	C	615	8CT	C14-C13	3.80	1.55	1.43
24	3	309	CHL	CHC-C4B	3.80	1.47	1.39
24	q	309	CHL	C1D-ND	-3.80	1.33	1.37
24	r	306	CHL	CHC-C4B	3.80	1.47	1.39
25	9	314	CLA	C1D-ND	3.80	1.42	1.37
33	d	411	LMG	O7-C10	3.80	1.45	1.34
24	G	313	CHL	CHC-C4B	3.80	1.47	1.39
24	9	305	CHL	CHC-C4B	3.79	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	316	CLA	C1D-ND	3.79	1.42	1.37
24	R	601	CHL	CHD-C4C	3.79	1.47	1.39
26	G	303	0IE	C11-C12	3.79	1.40	1.35
24	4	317	CHL	OBD-CAD	3.79	1.29	1.22
25	n	316	CLA	C1D-ND	3.79	1.42	1.37
24	5	311	CHL	CHC-C4B	3.79	1.47	1.39
25	A	610	CLA	C1D-ND	3.79	1.42	1.37
24	6	308	CHL	OBD-CAD	3.79	1.29	1.22
24	1	310	CHL	CHC-C4B	3.79	1.47	1.39
24	q	316	CHL	CHD-C4C	3.79	1.47	1.39
31	S	614	8CT	C28-C29	3.79	1.41	1.32
24	8	307	CHL	CHC-C4B	3.78	1.47	1.39
26	G	303	0IE	C15-C16	3.78	1.40	1.35
25	3	314	CLA	C1D-ND	3.78	1.42	1.37
26	7	303	0IE	C11-C12	3.78	1.40	1.35
24	5	309	CHL	CHD-C4C	3.78	1.47	1.39
25	u	316	CLA	C1D-ND	3.78	1.42	1.37
26	R	614	0IE	C15-C16	3.78	1.40	1.35
24	u	305	CHL	CHC-C4B	3.78	1.47	1.39
24	3	310	CHL	CHD-C4C	3.78	1.47	1.39
26	g	303	0IE	C15-C16	3.78	1.40	1.35
24	Y	304	CHL	CHC-C1C	3.78	1.46	1.38
25	u	315	CLA	C1D-ND	3.78	1.42	1.37
33	C	618	LMG	O7-C10	3.78	1.45	1.34
26	7	303	0IE	C15-C16	3.78	1.40	1.35
33	W	201	LMG	O7-C10	3.78	1.45	1.34
24	G	312	CHL	CHC-C4B	3.78	1.47	1.39
26	g	303	0IE	C8-C7	3.78	1.40	1.35
33	W	201	LMG	O8-C28	3.78	1.44	1.33
25	6	314	CLA	C1D-ND	3.77	1.42	1.37
24	g	311	CHL	CHC-C4B	3.77	1.47	1.39
24	8	303	CHL	CHD-C4C	3.77	1.47	1.39
24	r	309	CHL	C1D-ND	-3.77	1.33	1.37
24	q	303	CHL	CHD-C4C	3.77	1.47	1.39
24	2	313	CHL	C3A-C2A	-3.77	1.51	1.54
37	C	619	DGD	O2G-C1B	3.77	1.44	1.34
37	c	618	DGD	O2G-C1B	3.77	1.44	1.34
25	1	315	CLA	C1D-ND	3.77	1.42	1.37
24	n	308	CHL	CHD-C4C	3.77	1.47	1.39
24	p	318	CHL	CHC-C4B	3.77	1.47	1.39
24	1	308	CHL	OBD-CAD	3.77	1.29	1.22
26	G	303	0IE	C8-C7	3.77	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	u	307	CLA	C1D-ND	3.77	1.42	1.37
24	p	311	CHL	CHC-C4B	3.77	1.47	1.39
24	7	318	CHL	CHC-C4B	3.76	1.47	1.39
25	3	315	CLA	C1D-ND	3.76	1.42	1.37
31	c	613	8CT	C14-C13	3.76	1.55	1.43
24	2	318	CHL	CHD-C4C	3.76	1.47	1.39
24	q	307	CHL	CHC-C4B	3.76	1.47	1.39
25	9	315	CLA	C1D-ND	3.76	1.42	1.37
24	u	309	CHL	OBD-CAD	3.76	1.29	1.22
24	3	310	CHL	OBD-CAD	3.76	1.29	1.22
24	q	308	CHL	CHC-C4B	3.76	1.47	1.39
26	3	302	0IE	C15-C16	3.76	1.40	1.35
25	4	314	CLA	C1D-ND	3.76	1.42	1.37
24	9	309	CHL	CHD-C4C	3.76	1.47	1.39
25	G	307	CLA	C1D-ND	3.76	1.42	1.37
24	g	309	CHL	OBD-CAD	3.76	1.29	1.22
24	8	310	CHL	C1D-ND	-3.76	1.33	1.37
24	6	317	CHL	CHD-C4C	3.76	1.47	1.39
25	1	314	CLA	C1D-ND	3.76	1.42	1.37
24	n	304	CHL	OBD-CAD	3.75	1.28	1.22
24	2	309	CHL	CHD-C4C	3.75	1.47	1.39
25	g	307	CLA	C1D-ND	3.75	1.42	1.37
24	r	302	CHL	CHD-C4C	3.75	1.47	1.39
25	4	307	CLA	C1D-ND	3.75	1.42	1.37
25	9	313	CLA	C1D-ND	3.75	1.42	1.37
24	4	308	CHL	OBD-CAD	3.75	1.28	1.22
31	C	613	8CT	C14-C13	3.75	1.55	1.43
24	y	306	CHL	C1D-ND	-3.75	1.33	1.37
25	9	307	CLA	C1D-ND	3.75	1.42	1.37
24	9	308	CHL	OBD-CAD	3.75	1.28	1.22
24	6	310	CHL	OBD-CAD	3.75	1.28	1.22
26	q	302	0IE	C11-C12	3.75	1.40	1.35
24	8	303	CHL	CHC-C4B	3.75	1.47	1.39
24	S	602	CHL	OBD-CAD	3.75	1.28	1.22
24	R	608	CHL	C1D-ND	-3.75	1.33	1.37
24	8	304	CHL	C1D-ND	-3.75	1.33	1.37
25	G	315	CLA	C1D-ND	3.75	1.42	1.37
24	N	310	CHL	CHD-C4C	3.75	1.47	1.39
24	g	312	CHL	CHC-C4B	3.74	1.47	1.39
24	3	309	CHL	CHD-C4C	3.74	1.47	1.39
24	3	311	CHL	CHC-C4B	3.74	1.47	1.39
24	6	311	CHL	CHC-C4B	3.74	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	311	CHL	CHD-C4C	3.74	1.47	1.39
24	q	303	CHL	CHC-C4B	3.74	1.47	1.39
24	u	305	CHL	OBD-CAD	3.74	1.28	1.22
24	9	310	CHL	CHD-C4C	3.74	1.47	1.39
25	6	306	CLA	C1D-ND	3.74	1.42	1.37
24	g	310	CHL	OBD-CAD	3.74	1.28	1.22
26	p	303	0IE	C11-C12	3.74	1.40	1.35
24	3	317	CHL	CHD-C4C	3.74	1.47	1.39
24	q	304	CHL	C1D-ND	-3.74	1.33	1.37
24	9	304	CHL	CHD-C4C	3.74	1.47	1.39
24	g	312	CHL	CHD-C4C	3.74	1.47	1.39
24	G	309	CHL	OBD-CAD	3.74	1.28	1.22
33	D	401	LMG	O7-C10	3.74	1.44	1.34
24	5	311	CHL	CHD-C4C	3.74	1.47	1.39
24	N	308	CHL	CHC-C4B	3.73	1.47	1.39
24	5	318	CHL	CHD-C4C	3.73	1.47	1.39
31	t	101	8CT	C14-C13	3.73	1.55	1.43
24	3	308	CHL	OBD-CAD	3.73	1.28	1.22
25	6	313	CLA	C1D-ND	3.73	1.42	1.37
24	9	317	CHL	OBD-CAD	3.73	1.28	1.22
24	u	311	CHL	CHD-C4C	3.73	1.47	1.39
25	3	307	CLA	C1D-ND	3.73	1.42	1.37
31	v	401	8CT	C14-C13	3.73	1.55	1.43
33	D	411	LMG	O7-C10	3.73	1.44	1.34
24	6	304	CHL	CHC-C4B	3.73	1.47	1.39
24	6	309	CHL	CHD-C4C	3.73	1.47	1.39
24	G	312	CHL	CHD-C4C	3.73	1.47	1.39
26	Y	302	0IE	C11-C12	3.73	1.40	1.35
24	2	310	CHL	CHC-C4B	3.73	1.47	1.39
24	S	606	CHL	CHC-C4B	3.73	1.47	1.39
24	g	305	CHL	CHC-C4B	3.72	1.47	1.39
25	n	314	CLA	C1D-ND	3.72	1.42	1.37
24	G	306	CHL	CHC-C4B	3.72	1.47	1.39
24	y	305	CHL	CHC-C1C	3.72	1.46	1.38
24	3	309	CHL	OBD-CAD	3.72	1.28	1.22
37	C	620	DGD	O2G-C1B	3.72	1.44	1.34
26	2	302	0IE	C11-C12	3.72	1.40	1.35
24	G	311	CHL	CHC-C4B	3.72	1.47	1.39
24	4	317	CHL	CHB-C1B	3.72	1.47	1.39
31	V	401	8CT	C14-C13	3.72	1.55	1.43
31	T	101	8CT	C14-C13	3.72	1.55	1.43
25	g	314	CLA	C1D-ND	3.72	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	311	CHL	CHD-C4C	3.72	1.47	1.39
24	N	317	CHL	OBD-CAD	3.72	1.28	1.22
24	2	305	CHL	CHC-C4B	3.72	1.47	1.39
24	7	310	CHL	CHD-C4C	3.72	1.47	1.39
24	q	307	CHL	C1D-ND	-3.72	1.33	1.37
24	N	304	CHL	OBD-CAD	3.72	1.28	1.22
24	u	318	CHL	OBD-CAD	3.72	1.28	1.22
24	8	307	CHL	C1D-ND	-3.72	1.33	1.37
25	6	307	CLA	C1D-ND	3.72	1.42	1.37
24	1	312	CHL	CHC-C4B	3.71	1.47	1.39
24	g	318	CHL	CHC-C4B	3.71	1.47	1.39
24	Y	319	CHL	C1D-ND	-3.71	1.33	1.37
24	s	403	CHL	OBD-CAD	3.71	1.28	1.22
25	6	315	CLA	C1D-ND	3.71	1.42	1.37
28	6	303	NEX	C7-C8	-3.71	1.25	1.32
24	1	312	CHL	OBD-CAD	3.71	1.28	1.22
33	d	401	LMG	O7-C10	3.71	1.44	1.34
24	y	310	CHL	CHC-C4B	3.71	1.47	1.39
25	6	316	CLA	C1D-ND	3.71	1.42	1.37
24	G	318	CHL	CHC-C4B	3.71	1.47	1.39
24	4	312	CHL	CHC-C4B	3.71	1.47	1.39
24	n	317	CHL	OBD-CAD	3.71	1.28	1.22
24	9	309	CHL	OBD-CAD	3.71	1.28	1.22
24	5	313	CHL	C3A-C2A	-3.71	1.51	1.54
25	3	306	CLA	C1D-ND	3.71	1.42	1.37
24	N	308	CHL	OBD-CAD	3.71	1.28	1.22
25	r	312	CLA	C1D-ND	3.71	1.42	1.37
24	N	311	CHL	CHC-C4B	3.71	1.47	1.39
24	7	309	CHL	OBD-CAD	3.71	1.28	1.22
24	6	304	CHL	CHD-C4C	3.71	1.47	1.39
24	7	313	CHL	C1D-ND	-3.70	1.33	1.37
25	G	314	CLA	C1D-ND	3.70	1.42	1.37
25	4	306	CLA	C1D-ND	3.70	1.42	1.37
24	G	305	CHL	CHC-C4B	3.70	1.47	1.39
24	q	304	CHL	CHC-C4B	3.70	1.47	1.39
24	9	312	CHL	OBD-CAD	3.70	1.28	1.22
24	q	308	CHL	C1D-ND	-3.70	1.33	1.37
25	9	306	CLA	C1D-ND	3.70	1.42	1.37
24	G	306	CHL	OBD-CAD	3.70	1.28	1.22
24	4	312	CHL	OBD-CAD	3.70	1.28	1.22
24	8	308	CHL	CHC-C4B	3.70	1.47	1.39
24	6	309	CHL	OBD-CAD	3.70	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	608	8CT	C14-C13	3.70	1.54	1.43
24	2	311	CHL	CHD-C4C	3.70	1.47	1.39
25	4	313	CLA	C1D-ND	3.70	1.42	1.37
28	s	401	NEX	C7-C8	-3.70	1.25	1.32
26	7	303	0IE	C8-C7	3.70	1.40	1.35
25	2	308	CLA	C1D-ND	3.70	1.42	1.37
24	n	308	CHL	OBD-CAD	3.70	1.28	1.22
25	5	307	CLA	C1D-ND	3.70	1.42	1.37
24	5	306	CHL	OBD-CAD	3.70	1.28	1.22
24	2	313	CHL	CHD-C4C	3.70	1.47	1.39
24	5	313	CHL	CHD-C4C	3.69	1.47	1.39
24	8	315	CHL	OBD-CAD	3.69	1.28	1.22
24	r	307	CHL	OBD-CAD	3.69	1.28	1.22
24	q	311	CHL	C1D-ND	-3.69	1.33	1.37
24	u	310	CHL	OBD-CAD	3.69	1.28	1.22
26	y	302	0IE	C11-C12	3.69	1.40	1.35
31	C	614	8CT	C14-C13	3.69	1.54	1.43
24	G	310	CHL	OBD-CAD	3.69	1.28	1.22
31	B	617	8CT	C14-C13	3.69	1.54	1.43
24	N	312	CHL	CHD-C4C	3.69	1.47	1.39
24	g	306	CHL	CHC-C4B	3.69	1.47	1.39
24	p	310	CHL	CHD-C4C	3.69	1.47	1.39
25	N	314	CLA	C1D-ND	3.69	1.42	1.37
25	g	315	CLA	C1D-ND	3.69	1.42	1.37
24	R	606	CHL	OBD-CAD	3.69	1.28	1.22
24	g	311	CHL	OBD-CAD	3.69	1.28	1.22
24	p	305	CHL	OBD-CAD	3.69	1.28	1.22
24	n	311	CHL	CHC-C4B	3.69	1.47	1.39
24	n	310	CHL	CHD-C4C	3.69	1.47	1.39
24	3	317	CHL	OBD-CAD	3.69	1.28	1.22
24	9	304	CHL	CHC-C4B	3.69	1.47	1.39
24	Y	319	CHL	CHC-C4B	3.69	1.47	1.39
31	C	615	8CT	C11-C12	3.69	1.53	1.45
24	9	304	CHL	OBD-CAD	3.69	1.28	1.22
24	s	407	CHL	CHC-C4B	3.69	1.47	1.39
31	t	101	8CT	C30-C29	3.69	1.55	1.50
24	5	313	CHL	CHC-C4B	3.69	1.47	1.39
25	u	317	CLA	C1D-ND	3.69	1.42	1.37
31	b	617	8CT	C14-C13	3.69	1.54	1.43
24	r	309	CHL	OBD-CAD	3.69	1.28	1.22
24	2	313	CHL	CHC-C4B	3.69	1.47	1.39
24	8	304	CHL	CHC-C4B	3.69	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	403	CHL	CHC-C4B	3.69	1.47	1.39
33	m	101	LMG	O7-C10	3.68	1.44	1.34
24	1	304	CHL	OBD-CAD	3.68	1.28	1.22
24	g	306	CHL	OBD-CAD	3.68	1.28	1.22
31	T	101	8CT	C30-C29	3.68	1.55	1.50
26	2	302	0IE	C15-C16	3.68	1.40	1.35
24	5	305	CHL	OBD-CAD	3.68	1.28	1.22
24	n	312	CHL	CHD-C4C	3.68	1.47	1.39
24	1	310	CHL	OBD-CAD	3.68	1.28	1.22
24	4	304	CHL	OBD-CAD	3.68	1.28	1.22
24	Y	305	CHL	C1D-ND	-3.68	1.33	1.37
24	N	317	CHL	CHB-C1B	3.68	1.47	1.39
24	3	304	CHL	OBD-CAD	3.68	1.28	1.22
31	c	614	8CT	C14-C13	3.68	1.54	1.43
24	8	308	CHL	C1D-ND	-3.68	1.33	1.37
24	S	602	CHL	CHC-C4B	3.68	1.47	1.39
25	n	306	CLA	C1D-ND	3.68	1.42	1.37
26	5	302	0IE	C11-C12	3.68	1.40	1.35
25	R	611	CLA	C1D-ND	3.68	1.42	1.37
25	q	315	CLA	C1D-ND	3.68	1.42	1.37
24	q	316	CHL	OBD-CAD	3.68	1.28	1.22
33	i	101	LMG	O7-C10	3.68	1.44	1.34
24	4	309	CHL	OBD-CAD	3.68	1.28	1.22
25	r	313	CLA	C1D-ND	3.68	1.42	1.37
24	4	310	CHL	OBD-CAD	3.68	1.28	1.22
24	4	312	CHL	C1D-ND	-3.68	1.33	1.37
24	p	313	CHL	C1D-ND	-3.68	1.33	1.37
25	3	313	CLA	C1D-ND	3.68	1.42	1.37
24	p	310	CHL	C1D-ND	-3.67	1.33	1.37
25	r	314	CLA	C4B-NB	3.67	1.42	1.37
24	p	309	CHL	OBD-CAD	3.67	1.28	1.22
31	A	608	8CT	C14-C13	3.67	1.54	1.43
26	8	302	0IE	C11-C12	3.67	1.40	1.35
24	s	414	CHL	C1D-ND	-3.67	1.33	1.37
24	5	305	CHL	CHD-C4C	3.67	1.47	1.39
25	G	308	CLA	C1D-ND	3.67	1.42	1.37
25	N	306	CLA	C1D-ND	3.67	1.42	1.37
24	Y	308	CHL	CHC-C4B	3.67	1.47	1.39
25	8	314	CLA	C1D-ND	3.67	1.42	1.37
24	1	305	CHL	CHC-C4B	3.67	1.47	1.39
31	B	617	8CT	C11-C12	3.67	1.53	1.45
24	9	311	CHL	CHD-C4C	3.67	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	316	CLA	C1D-ND	3.67	1.42	1.37
24	3	304	CHL	CHD-C4C	3.67	1.47	1.39
24	R	608	CHL	OBD-CAD	3.67	1.28	1.22
26	5	302	0IE	C8-C7	3.67	1.40	1.35
25	u	308	CLA	C1D-ND	3.67	1.42	1.37
24	7	310	CHL	C1D-ND	-3.67	1.33	1.37
24	1	317	CHL	CHB-C1B	3.67	1.47	1.39
24	G	318	CHL	OBD-CAD	3.67	1.28	1.22
24	s	414	CHL	CHC-C4B	3.66	1.47	1.39
24	p	306	CHL	C1D-ND	-3.66	1.33	1.37
25	1	306	CLA	C1D-ND	3.66	1.42	1.37
24	r	303	CHL	OBD-CAD	3.66	1.28	1.22
31	D	410	8CT	C14-C13	3.66	1.54	1.43
25	p	308	CLA	C1D-ND	3.66	1.42	1.37
24	s	402	CHL	CHC-C4B	3.66	1.47	1.39
25	1	307	CLA	C1D-ND	3.66	1.42	1.37
24	2	306	CHL	OBD-CAD	3.66	1.28	1.22
24	G	313	CHL	OBD-CAD	3.66	1.28	1.22
24	6	317	CHL	OBD-CAD	3.66	1.28	1.22
24	g	305	CHL	OBD-CAD	3.66	1.28	1.22
28	n	303	NEX	C7-C8	-3.66	1.25	1.32
24	6	304	CHL	OBD-CAD	3.66	1.28	1.22
24	4	305	CHL	CHC-C4B	3.66	1.47	1.39
24	5	305	CHL	CHC-C4B	3.66	1.47	1.39
24	R	605	CHL	CHC-C4B	3.66	1.47	1.39
24	n	312	CHL	CHC-C4B	3.66	1.47	1.39
24	r	302	CHL	OBD-CAD	3.66	1.28	1.22
24	N	312	CHL	CHC-C4B	3.66	1.47	1.39
24	5	310	CHL	CHC-C4B	3.66	1.47	1.39
31	t	101	8CT	C28-C29	3.66	1.40	1.32
24	4	312	CHL	CHD-C4C	3.66	1.47	1.39
24	S	613	CHL	CHC-C4B	3.66	1.47	1.39
24	Y	309	CHL	CHC-C4B	3.66	1.47	1.39
24	2	305	CHL	CHD-C4C	3.66	1.47	1.39
25	R	612	CLA	C1D-ND	3.66	1.42	1.37
24	R	602	CHL	OBD-CAD	3.66	1.28	1.22
24	4	311	CHL	CHD-C4C	3.65	1.47	1.39
24	S	605	CHL	CHC-C4B	3.65	1.47	1.39
24	g	305	CHL	CHD-C4C	3.65	1.47	1.39
24	n	309	CHL	OBD-CAD	3.65	1.28	1.22
31	d	410	8CT	C14-C13	3.65	1.54	1.43
24	R	605	CHL	OBD-CAD	3.65	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	309	CHL	CHC-C4B	3.65	1.47	1.39
31	c	615	8CT	C11-C12	3.65	1.53	1.45
24	Y	317	CHL	C1D-ND	-3.65	1.33	1.37
24	1	312	CHL	CHD-C4C	3.65	1.47	1.39
24	G	309	CHL	CHB-C1B	3.65	1.47	1.39
24	9	308	CHL	CHB-C1B	3.65	1.47	1.39
24	7	306	CHL	C1D-ND	-3.65	1.33	1.37
25	2	317	CLA	C1D-ND	3.65	1.42	1.37
25	r	311	CLA	C1D-ND	3.65	1.42	1.37
28	r	301	NEX	C7-C8	-3.65	1.25	1.32
24	5	311	CHL	C1D-ND	-3.65	1.33	1.37
28	3	318	NEX	C7-C8	-3.65	1.25	1.32
24	1	304	CHL	CHB-C1B	3.65	1.47	1.39
25	3	316	CLA	C1D-ND	3.65	1.42	1.37
24	1	311	CHL	CHC-C4B	3.65	1.47	1.39
24	N	308	CHL	CHD-C4C	3.65	1.47	1.39
31	T	101	8CT	C28-C29	3.65	1.40	1.32
24	5	306	CHL	CHC-C4B	3.65	1.47	1.39
24	N	310	CHL	OBD-CAD	3.65	1.28	1.22
25	r	310	CLA	C1D-ND	3.64	1.42	1.37
24	u	312	CHL	CHD-C4C	3.64	1.47	1.39
24	n	317	CHL	CHB-C1B	3.64	1.47	1.39
24	G	318	CHL	CHD-C4C	3.64	1.47	1.39
24	r	307	CHL	C1D-ND	-3.64	1.33	1.37
25	1	313	CLA	C1D-ND	3.64	1.42	1.37
25	8	312	CLA	C1D-ND	3.64	1.42	1.37
24	G	305	CHL	OBD-CAD	3.64	1.28	1.22
25	g	317	CLA	C1D-ND	3.64	1.42	1.37
25	5	308	CLA	C1D-ND	3.64	1.42	1.37
24	g	313	CHL	OBD-CAD	3.64	1.28	1.22
24	g	318	CHL	CHD-C4C	3.64	1.47	1.39
25	R	613	CLA	C4B-NB	3.64	1.42	1.37
24	2	310	CHL	OBD-CAD	3.64	1.28	1.22
24	7	305	CHL	OBD-CAD	3.64	1.28	1.22
31	x	601	8CT	C14-C13	3.64	1.54	1.43
24	S	613	CHL	C1D-ND	-3.64	1.33	1.37
31	s	416	8CT	C30-C29	3.64	1.55	1.50
26	2	302	0IE	C8-C7	3.64	1.40	1.35
24	n	310	CHL	OBD-CAD	3.64	1.28	1.22
24	G	305	CHL	CHD-C4C	3.64	1.47	1.39
24	3	304	CHL	CHC-C4B	3.64	1.47	1.39
24	4	311	CHL	CHC-C4B	3.64	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	316	CLA	C1D-ND	3.64	1.42	1.37
24	9	305	CHL	OBD-CAD	3.64	1.28	1.22
25	g	308	CLA	C1D-ND	3.64	1.42	1.37
24	3	312	CHL	CHB-C1B	3.63	1.47	1.39
30	d	408	LHG	O7-C7	3.63	1.44	1.34
24	S	601	CHL	CHC-C4B	3.63	1.47	1.39
33	B	619	LMG	O7-C10	3.63	1.44	1.34
24	2	305	CHL	OBD-CAD	3.63	1.28	1.22
31	X	601	8CT	C14-C13	3.63	1.54	1.43
24	R	601	CHL	OBD-CAD	3.63	1.28	1.22
24	r	306	CHL	OBD-CAD	3.63	1.28	1.22
24	g	313	CHL	CHB-C1B	3.63	1.47	1.39
24	1	309	CHL	OBD-CAD	3.63	1.28	1.22
24	5	313	CHL	C1D-ND	-3.63	1.33	1.37
24	5	318	CHL	OBD-CAD	3.63	1.28	1.22
24	5	311	CHL	OBD-CAD	3.63	1.28	1.22
24	2	306	CHL	CHC-C4B	3.63	1.47	1.39
24	n	310	CHL	C1D-ND	-3.63	1.33	1.37
24	Y	308	CHL	C1D-ND	-3.63	1.33	1.37
24	g	318	CHL	OBD-CAD	3.63	1.28	1.22
24	7	310	CHL	OBD-CAD	3.63	1.28	1.22
26	y	303	0IE	C11-C12	3.63	1.40	1.35
24	g	309	CHL	CHB-C1B	3.62	1.47	1.39
24	s	406	CHL	CHC-C4B	3.62	1.47	1.39
31	C	613	8CT	C11-C12	3.62	1.53	1.45
24	4	304	CHL	CHB-C1B	3.62	1.47	1.39
24	S	607	CHL	OBD-CAD	3.62	1.28	1.22
24	p	318	CHL	CHD-C4C	3.62	1.47	1.39
24	5	310	CHL	OBD-CAD	3.62	1.28	1.22
26	Y	303	0IE	C11-C12	3.62	1.40	1.35
24	g	312	CHL	OBD-CAD	3.62	1.28	1.22
24	G	311	CHL	OBD-CAD	3.62	1.28	1.22
24	r	303	CHL	C1D-ND	-3.62	1.33	1.37
24	G	306	CHL	CHD-C4C	3.62	1.47	1.39
26	5	302	0IE	C15-C16	3.62	1.40	1.35
24	y	313	CHL	C1D-ND	-3.62	1.33	1.37
24	q	303	CHL	OBD-CAD	3.62	1.28	1.22
24	u	309	CHL	CHB-C1B	3.62	1.47	1.39
37	c	619	DGD	O2G-C1B	3.62	1.44	1.34
26	Y	303	0IE	C8-C7	3.62	1.40	1.35
25	S	603	CLA	C1D-ND	3.62	1.42	1.37
24	9	305	CHL	CHD-C4C	3.62	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	606	CHL	C1D-ND	-3.62	1.33	1.37
26	p	303	0IE	C8-C7	3.62	1.40	1.35
24	p	310	CHL	OBD-CAD	3.62	1.28	1.22
24	1	312	CHL	C1D-ND	-3.62	1.33	1.37
25	G	317	CLA	C1D-ND	3.62	1.42	1.37
24	s	409	CHL	CHD-C4C	3.62	1.47	1.39
24	p	312	CHL	CHC-C4B	3.62	1.47	1.39
24	u	310	CHL	CHB-C1B	3.62	1.47	1.39
24	y	318	CHL	C1D-ND	-3.62	1.33	1.37
25	n	315	CLA	C1D-ND	3.62	1.42	1.37
24	1	311	CHL	CHD-C4C	3.61	1.47	1.39
24	S	608	CHL	CHD-C4C	3.61	1.47	1.39
24	r	307	CHL	CHC-C4B	3.61	1.47	1.39
24	7	306	CHL	CHC-C4B	3.61	1.47	1.39
25	q	313	CLA	C1D-ND	3.61	1.42	1.37
31	S	615	8CT	C30-C29	3.61	1.55	1.50
25	N	315	CLA	C1D-ND	3.61	1.42	1.37
24	p	318	CHL	OBD-CAD	3.61	1.28	1.22
24	s	407	CHL	OBD-CAD	3.61	1.28	1.22
24	3	312	CHL	OBD-CAD	3.61	1.28	1.22
24	y	313	CHL	CHD-C4C	3.61	1.47	1.39
24	1	308	CHL	CHB-C1B	3.61	1.47	1.39
24	1	311	CHL	OBD-CAD	3.61	1.28	1.22
28	N	303	NEX	C7-C8	-3.61	1.25	1.32
24	N	312	CHL	OBD-CAD	3.61	1.28	1.22
24	y	309	CHL	CHC-C4B	3.61	1.47	1.39
24	2	313	CHL	OBD-CAD	3.61	1.28	1.22
24	8	315	CHL	CHB-C1B	3.61	1.47	1.39
24	p	306	CHL	CHC-C4B	3.61	1.47	1.39
24	y	309	CHL	C1D-ND	-3.61	1.33	1.37
24	9	310	CHL	OBD-CAD	3.61	1.28	1.22
24	u	306	CHL	CHD-C4C	3.61	1.47	1.39
24	n	312	CHL	OBD-CAD	3.61	1.28	1.22
31	b	617	8CT	C11-C12	3.61	1.53	1.45
24	N	305	CHL	C1D-ND	-3.61	1.33	1.37
24	5	318	CHL	C3A-C2A	-3.61	1.51	1.54
24	p	309	CHL	CHB-C1B	3.61	1.47	1.39
24	y	318	CHL	CHC-C4B	3.60	1.47	1.39
24	N	310	CHL	C1D-ND	-3.60	1.33	1.37
24	6	312	CHL	OBD-CAD	3.60	1.28	1.22
25	r	304	CLA	C1D-ND	3.60	1.42	1.37
24	8	303	CHL	OBD-CAD	3.60	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	307	CHL	CHD-C4C	3.60	1.47	1.39
24	q	316	CHL	CHB-C1B	3.60	1.47	1.39
24	N	311	CHL	OBD-CAD	3.60	1.28	1.22
24	3	305	CHL	C1D-ND	-3.60	1.33	1.37
24	3	305	CHL	CHD-C4C	3.60	1.47	1.39
24	q	307	CHL	CHD-C4C	3.60	1.47	1.39
24	7	318	CHL	CHD-C4C	3.60	1.47	1.39
24	4	310	CHL	CHD-C4C	3.60	1.47	1.39
24	Y	308	CHL	CHD-C4C	3.60	1.47	1.39
25	2	307	CLA	C1D-ND	3.60	1.42	1.37
24	1	305	CHL	OBD-CAD	3.60	1.28	1.22
24	r	309	CHL	CHC-C4B	3.60	1.47	1.39
24	4	308	CHL	CHB-C1B	3.60	1.47	1.39
24	u	306	CHL	OBD-CAD	3.60	1.28	1.22
24	y	305	CHL	C1D-ND	-3.60	1.33	1.37
24	9	317	CHL	CHB-C1B	3.60	1.47	1.39
24	q	308	CHL	OBD-CAD	3.60	1.28	1.22
24	y	311	CHL	OBD-CAD	3.59	1.28	1.22
24	Y	312	CHL	C1D-ND	-3.59	1.33	1.37
24	r	306	CHL	CHD-C4C	3.59	1.47	1.39
24	5	312	CHL	CHC-C4B	3.59	1.47	1.39
24	Y	304	CHL	C1D-ND	-3.59	1.33	1.37
25	R	610	CLA	C1D-ND	3.59	1.42	1.37
24	s	409	CHL	OBD-CAD	3.59	1.28	1.22
24	2	312	CHL	CHC-C4B	3.59	1.47	1.39
25	r	305	CLA	C1D-ND	3.59	1.42	1.37
24	7	313	CHL	CHD-C4C	3.59	1.47	1.39
24	S	606	CHL	OBD-CAD	3.59	1.28	1.22
24	n	311	CHL	OBD-CAD	3.59	1.28	1.22
24	G	310	CHL	CHB-C1B	3.59	1.47	1.39
26	y	302	0IE	C8-C7	3.59	1.40	1.35
24	R	606	CHL	CHC-C4B	3.59	1.47	1.39
24	8	309	CHL	C1D-ND	-3.59	1.33	1.37
25	5	316	CLA	C1D-ND	3.59	1.42	1.37
24	s	406	CHL	OBD-CAD	3.59	1.28	1.22
25	N	307	CLA	C1D-ND	3.59	1.42	1.37
25	5	315	CLA	C1D-ND	3.59	1.42	1.37
25	7	308	CLA	C1D-ND	3.59	1.42	1.37
24	u	312	CHL	OBD-CAD	3.59	1.28	1.22
24	7	318	CHL	OBD-CAD	3.59	1.28	1.22
24	q	307	CHL	OBD-CAD	3.59	1.28	1.22
26	8	302	0IE	C8-C7	3.59	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	604	CLA	C1D-ND	3.59	1.42	1.37
24	6	312	CHL	CHB-C1B	3.59	1.47	1.39
24	u	313	CHL	OBD-CAD	3.59	1.28	1.22
24	2	313	CHL	C1D-ND	-3.59	1.33	1.37
24	g	310	CHL	CHB-C1B	3.59	1.47	1.39
24	u	313	CHL	CHB-C1B	3.59	1.47	1.39
24	7	309	CHL	CHB-C1B	3.59	1.47	1.39
24	y	309	CHL	CHD-C4C	3.59	1.47	1.39
25	R	609	CLA	C1D-ND	3.59	1.42	1.37
24	6	311	CHL	CHD-C4C	3.59	1.47	1.39
24	p	311	CHL	OBD-CAD	3.59	1.28	1.22
24	5	309	CHL	C1D-ND	-3.59	1.33	1.37
25	R	603	CLA	C1D-ND	3.59	1.42	1.37
24	2	309	CHL	OBD-CAD	3.59	1.28	1.22
24	y	309	CHL	OBD-CAD	3.59	1.28	1.22
25	B	606	CLA	C4D-ND	-3.58	1.32	1.37
24	N	305	CHL	OBD-CAD	3.58	1.28	1.22
24	4	305	CHL	OBD-CAD	3.58	1.28	1.22
24	4	311	CHL	OBD-CAD	3.58	1.28	1.22
31	B	617	8CT	C28-C29	3.58	1.40	1.32
25	G	316	CLA	C1D-ND	3.58	1.42	1.37
26	Y	302	0IE	C15-C16	3.58	1.40	1.35
24	8	307	CHL	OBD-CAD	3.58	1.28	1.22
24	3	311	CHL	OBD-CAD	3.58	1.28	1.22
24	2	311	CHL	OBD-CAD	3.58	1.28	1.22
24	Y	310	CHL	CHC-C4B	3.58	1.47	1.39
24	1	310	CHL	CHD-C4C	3.58	1.47	1.39
24	2	311	CHL	C1D-ND	-3.58	1.33	1.37
24	n	305	CHL	OBD-CAD	3.58	1.28	1.22
24	6	308	CHL	CHB-C1B	3.58	1.47	1.39
24	u	318	CHL	CHB-C1B	3.58	1.47	1.39
26	q	302	0IE	C8-C7	3.58	1.40	1.35
24	2	306	CHL	C1D-ND	-3.58	1.33	1.37
24	y	311	CHL	CHC-C4B	3.58	1.47	1.39
24	s	414	CHL	OBD-CAD	3.58	1.28	1.22
26	Y	302	0IE	C8-C7	3.58	1.40	1.35
24	s	407	CHL	CHD-C4C	3.58	1.47	1.39
24	1	309	CHL	CHB-C1B	3.58	1.47	1.39
24	Y	317	CHL	CHC-C4B	3.58	1.47	1.39
24	5	313	CHL	OBD-CAD	3.57	1.28	1.22
25	q	314	CLA	C1D-ND	3.57	1.42	1.37
31	c	613	8CT	C11-C12	3.57	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	u	311	CHL	OBD-CAD	3.57	1.28	1.22
24	3	308	CHL	CHB-C1B	3.57	1.47	1.39
24	7	312	CHL	CHC-C4B	3.57	1.47	1.39
24	R	602	CHL	C1D-ND	-3.57	1.33	1.37
31	v	401	8CT	C28-C29	3.57	1.40	1.32
24	r	303	CHL	CHC-C4B	3.57	1.47	1.39
24	R	608	CHL	CHC-C4B	3.57	1.47	1.39
24	S	608	CHL	OBD-CAD	3.57	1.28	1.22
24	9	312	CHL	CHB-C1B	3.57	1.47	1.39
24	3	311	CHL	CHD-C4C	3.57	1.47	1.39
24	Y	312	CHL	CHD-C4C	3.57	1.47	1.39
24	6	310	CHL	CHB-C1B	3.57	1.47	1.39
25	2	316	CLA	C1D-ND	3.57	1.42	1.37
24	p	313	CHL	CHD-C4C	3.57	1.47	1.39
24	Y	311	CHL	CHC-C4B	3.57	1.47	1.39
25	A	604	CLA	C4D-ND	-3.57	1.32	1.37
24	6	305	CHL	CHD-C4C	3.57	1.47	1.39
24	G	312	CHL	OBD-CAD	3.57	1.28	1.22
25	5	317	CLA	C1D-ND	3.57	1.42	1.37
26	y	303	0IE	C8-C7	3.57	1.40	1.35
24	n	305	CHL	C1D-ND	-3.57	1.33	1.37
25	B	604	CLA	C1D-ND	3.57	1.42	1.37
24	5	306	CHL	C1D-ND	-3.57	1.33	1.37
25	n	313	CLA	C1D-ND	3.57	1.42	1.37
24	n	308	CHL	CHB-C1B	3.56	1.47	1.39
24	y	313	CHL	CHC-C4B	3.56	1.47	1.39
24	S	601	CHL	C1D-ND	-3.56	1.33	1.37
25	2	314	CLA	C1D-ND	3.56	1.42	1.37
26	y	302	0IE	C15-C16	3.56	1.40	1.35
25	A	603	CLA	C4D-ND	-3.56	1.32	1.37
24	3	310	CHL	C1D-ND	-3.56	1.33	1.37
24	6	311	CHL	OBD-CAD	3.56	1.28	1.22
24	2	318	CHL	C3A-C2A	-3.56	1.51	1.54
24	4	309	CHL	CHB-C1B	3.56	1.47	1.39
24	s	406	CHL	C1D-ND	-3.56	1.33	1.37
25	5	314	CLA	C1D-ND	3.56	1.42	1.37
24	3	310	CHL	CHB-C1B	3.56	1.47	1.39
24	9	312	CHL	C1D-ND	-3.56	1.33	1.37
24	n	308	CHL	C1D-ND	-3.56	1.33	1.37
25	8	313	CLA	C1D-ND	3.56	1.42	1.37
24	y	305	CHL	OBD-CAD	3.56	1.28	1.22
24	9	309	CHL	CHB-C1B	3.56	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	305	CHL	C1D-ND	-3.56	1.33	1.37
24	1	305	CHL	CHD-C4C	3.55	1.47	1.39
24	3	309	CHL	CHB-C1B	3.55	1.47	1.39
24	5	309	CHL	OBD-CAD	3.55	1.28	1.22
24	y	312	CHL	CHC-C4B	3.55	1.47	1.39
24	7	311	CHL	C1D-ND	-3.55	1.33	1.37
25	p	314	CLA	C1D-ND	3.55	1.42	1.37
24	4	305	CHL	CHD-C4C	3.55	1.47	1.39
24	1	312	CHL	CHB-C1B	3.55	1.47	1.39
24	G	313	CHL	CHB-C1B	3.55	1.47	1.39
24	s	409	CHL	CHC-C4B	3.55	1.47	1.39
24	6	305	CHL	OBD-CAD	3.55	1.28	1.22
24	Y	312	CHL	CHC-C4B	3.55	1.47	1.39
24	R	601	CHL	C1D-ND	-3.55	1.33	1.37
24	q	309	CHL	OBD-CAD	3.55	1.28	1.22
24	8	308	CHL	OBD-CAD	3.55	1.28	1.22
24	S	605	CHL	CHD-C4C	3.55	1.47	1.39
24	u	306	CHL	C1D-ND	-3.55	1.33	1.37
25	N	313	CLA	C1D-ND	3.55	1.42	1.37
24	u	305	CHL	CHB-C1B	3.55	1.47	1.39
24	Y	308	CHL	OBD-CAD	3.55	1.28	1.22
24	s	406	CHL	CHD-C4C	3.54	1.47	1.39
31	c	614	8CT	C11-C12	3.54	1.53	1.45
24	2	318	CHL	OBD-CAD	3.54	1.28	1.22
24	g	306	CHL	CHD-C4C	3.54	1.47	1.39
25	p	317	CLA	C1D-ND	3.54	1.42	1.37
31	b	617	8CT	C28-C29	3.54	1.40	1.32
24	5	309	CHL	CHB-C1B	3.54	1.47	1.39
25	S	609	CLA	C1D-ND	3.54	1.42	1.37
25	7	314	CLA	C1D-ND	3.54	1.42	1.37
24	N	309	CHL	CHC-C4B	3.54	1.47	1.39
24	s	408	CHL	CHC-C4B	3.54	1.47	1.39
24	S	613	CHL	OBD-CAD	3.54	1.28	1.22
24	q	303	CHL	C1D-ND	-3.54	1.33	1.37
24	7	313	CHL	CHC-C4B	3.54	1.47	1.39
25	b	606	CLA	C4D-ND	-3.54	1.32	1.37
24	S	608	CHL	CHC-C4B	3.54	1.47	1.39
25	2	315	CLA	C1D-ND	3.54	1.42	1.37
24	Y	304	CHL	OBD-CAD	3.54	1.28	1.22
24	2	309	CHL	C1D-ND	-3.54	1.33	1.37
25	B	601	CLA	C1D-ND	3.53	1.42	1.37
24	8	310	CHL	CHD-C4C	3.53	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	311	CHL	OBD-CAD	3.53	1.28	1.22
24	5	312	CHL	OBD-CAD	3.53	1.28	1.22
24	p	311	CHL	CHD-C4C	3.53	1.47	1.39
24	R	602	CHL	CHC-C4B	3.53	1.47	1.39
31	V	401	8CT	C28-C29	3.53	1.40	1.32
24	Y	310	CHL	OBD-CAD	3.53	1.28	1.22
24	Y	319	CHL	OBD-CAD	3.53	1.28	1.22
24	S	605	CHL	OBD-CAD	3.53	1.28	1.22
24	q	304	CHL	OBD-CAD	3.53	1.28	1.22
24	N	308	CHL	C1D-ND	-3.53	1.33	1.37
24	S	606	CHL	CHD-C4C	3.53	1.47	1.39
24	u	311	CHL	CHB-C1B	3.53	1.47	1.39
24	9	310	CHL	CHB-C1B	3.53	1.47	1.39
24	8	303	CHL	C1D-ND	-3.53	1.33	1.37
25	s	404	CLA	C1D-ND	3.53	1.42	1.37
24	u	312	CHL	CHB-C1B	3.53	1.47	1.39
24	4	308	CHL	C1D-ND	-3.53	1.33	1.37
25	c	609	CLA	C4D-ND	-3.52	1.32	1.37
24	2	318	CHL	CHB-C1B	3.52	1.47	1.39
24	5	318	CHL	CHB-C1B	3.52	1.47	1.39
24	y	306	CHL	OBD-CAD	3.52	1.28	1.22
24	8	304	CHL	OBD-CAD	3.52	1.28	1.22
24	5	311	CHL	CHB-C1B	3.52	1.47	1.39
25	p	315	CLA	C1D-ND	3.52	1.42	1.37
24	S	607	CHL	CHC-C4B	3.52	1.47	1.39
24	q	310	CHL	CHC-C4B	3.52	1.47	1.39
24	s	402	CHL	OBD-CAD	3.52	1.28	1.22
31	C	614	8CT	C11-C12	3.52	1.53	1.45
24	y	310	CHL	C1D-ND	-3.52	1.33	1.37
25	7	315	CLA	C1D-ND	3.52	1.42	1.37
25	7	317	CLA	C1D-ND	3.52	1.42	1.37
24	q	311	CHL	CHD-C4C	3.52	1.47	1.39
24	7	311	CHL	CHD-C4C	3.52	1.47	1.39
25	b	601	CLA	C1D-ND	3.51	1.42	1.37
24	7	311	CHL	OBD-CAD	3.51	1.28	1.22
24	8	310	CHL	CHC-C4B	3.51	1.47	1.39
25	B	610	CLA	C4D-ND	-3.51	1.32	1.37
24	p	313	CHL	CHC-C4B	3.51	1.47	1.39
24	Y	309	CHL	OBD-CAD	3.51	1.28	1.22
24	2	311	CHL	CHB-C1B	3.51	1.47	1.39
24	S	606	CHL	C1D-ND	-3.51	1.33	1.37
24	2	318	CHL	C1D-ND	-3.51	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	310	CHL	C1D-ND	-3.51	1.33	1.37
25	c	602	CLA	C4D-ND	-3.51	1.32	1.37
24	s	402	CHL	C1D-ND	-3.51	1.33	1.37
24	8	309	CHL	OBD-CAD	3.51	1.28	1.22
24	g	311	CHL	CHB-C1B	3.51	1.47	1.39
24	2	312	CHL	OBD-CAD	3.51	1.28	1.22
31	x	601	8CT	C11-C12	3.51	1.53	1.45
31	X	601	8CT	C11-C12	3.51	1.53	1.45
24	2	310	CHL	C1D-ND	-3.51	1.33	1.37
31	c	615	8CT	C28-C29	3.51	1.40	1.32
25	a	604	CLA	C4D-ND	-3.51	1.32	1.37
24	2	313	CHL	CHB-C1B	3.51	1.47	1.39
24	6	309	CHL	CHB-C1B	3.51	1.47	1.39
31	d	410	8CT	C28-C29	3.51	1.40	1.32
24	9	305	CHL	C1D-ND	-3.50	1.33	1.37
25	s	410	CLA	C1D-ND	3.50	1.42	1.37
24	2	309	CHL	CHB-C1B	3.50	1.47	1.39
31	D	410	8CT	C28-C29	3.50	1.40	1.32
24	q	310	CHL	C1D-ND	-3.50	1.33	1.37
24	p	312	CHL	OBD-CAD	3.50	1.28	1.22
24	2	312	CHL	CHD-C4C	3.50	1.47	1.39
24	5	312	CHL	CHD-C4C	3.50	1.47	1.39
24	y	313	CHL	OBD-CAD	3.50	1.28	1.22
24	5	318	CHL	C1D-ND	-3.50	1.33	1.37
24	Y	305	CHL	OBD-CAD	3.50	1.28	1.22
25	C	609	CLA	C4D-ND	-3.50	1.32	1.37
24	G	312	CHL	CHB-C1B	3.50	1.47	1.39
31	t	101	8CT	C35-C30	3.50	1.66	1.56
24	p	311	CHL	C1D-ND	-3.50	1.33	1.37
24	p	313	CHL	OBD-CAD	3.50	1.28	1.22
24	u	310	CHL	C1D-ND	-3.50	1.33	1.37
24	3	305	CHL	OBD-CAD	3.50	1.28	1.22
24	N	309	CHL	OBD-CAD	3.50	1.28	1.22
25	n	307	CLA	C1D-ND	3.50	1.42	1.37
25	a	603	CLA	C4D-ND	-3.50	1.32	1.37
25	b	604	CLA	C1D-ND	3.50	1.42	1.37
24	S	607	CHL	CHD-C4C	3.50	1.47	1.39
25	D	404	CLA	C4D-ND	-3.49	1.32	1.37
24	q	311	CHL	CHC-C4B	3.49	1.47	1.39
25	d	404	CLA	C4D-ND	-3.49	1.32	1.37
25	c	607	CLA	C4D-ND	-3.49	1.32	1.37
31	C	615	8CT	C28-C29	3.49	1.40	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	309	CHL	CHC-C4B	3.49	1.47	1.39
24	r	302	CHL	C1D-ND	-3.49	1.33	1.37
24	y	310	CHL	OBD-CAD	3.49	1.28	1.22
24	6	310	CHL	C1D-ND	-3.49	1.33	1.37
24	3	317	CHL	CHB-C1B	3.48	1.47	1.39
24	1	310	CHL	C1D-ND	-3.48	1.33	1.37
24	Y	319	CHL	CHD-C4C	3.48	1.47	1.39
24	n	305	CHL	CHD-C4C	3.48	1.47	1.39
24	7	309	CHL	C3D-C2D	3.48	1.48	1.39
24	p	309	CHL	C3D-C2D	3.48	1.48	1.39
24	G	305	CHL	C1D-ND	-3.48	1.33	1.37
24	g	312	CHL	CHB-C1B	3.48	1.47	1.39
24	S	605	CHL	C1D-ND	-3.48	1.33	1.37
24	G	311	CHL	C1D-ND	-3.48	1.33	1.37
25	y	316	CLA	C4D-ND	-3.48	1.32	1.37
24	7	313	CHL	OBD-CAD	3.48	1.28	1.22
31	T	101	8CT	C35-C30	3.48	1.66	1.56
24	g	305	CHL	C1D-ND	-3.48	1.33	1.37
25	7	316	CLA	C1D-ND	3.48	1.42	1.37
31	d	410	8CT	C11-C12	3.48	1.53	1.45
24	N	304	CHL	CHB-C1B	3.48	1.47	1.39
24	8	309	CHL	CHC-C4B	3.48	1.47	1.39
24	7	310	CHL	CHB-C1B	3.48	1.47	1.39
24	S	601	CHL	OBD-CAD	3.48	1.28	1.22
24	7	318	CHL	C1D-ND	-3.48	1.33	1.37
31	D	410	8CT	C01-C02	3.48	1.56	1.50
24	s	407	CHL	C1D-ND	-3.48	1.33	1.37
25	C	610	CLA	C4D-ND	-3.48	1.32	1.37
31	D	410	8CT	C11-C12	3.48	1.53	1.45
24	2	310	CHL	CHD-C4C	3.47	1.47	1.39
24	s	402	CHL	CHD-C4C	3.47	1.47	1.39
24	r	306	CHL	C1D-ND	-3.47	1.33	1.37
24	5	313	CHL	CHB-C1B	3.47	1.47	1.39
24	N	311	CHL	CHD-C4C	3.47	1.47	1.39
24	6	317	CHL	CHB-C1B	3.47	1.47	1.39
24	4	310	CHL	C1D-ND	-3.47	1.33	1.37
24	R	607	CHL	OBD-CAD	3.47	1.28	1.22
24	Y	309	CHL	C1D-ND	-3.47	1.33	1.37
24	4	309	CHL	C1D-ND	-3.47	1.33	1.37
24	9	311	CHL	CHB-C1B	3.47	1.47	1.39
24	3	317	CHL	C1D-ND	-3.47	1.33	1.37
25	B	607	CLA	C1D-ND	3.47	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	307	CLA	C1D-ND	3.47	1.42	1.37
24	9	309	CHL	C1D-ND	-3.47	1.33	1.37
24	y	312	CHL	C1D-ND	-3.47	1.33	1.37
25	p	316	CLA	C1D-ND	3.47	1.42	1.37
26	8	302	0IE	C15-C16	3.47	1.40	1.35
24	u	313	CHL	C1D-ND	-3.47	1.33	1.37
25	S	604	CLA	C1D-ND	3.47	1.42	1.37
25	s	417	CLA	C1D-ND	3.47	1.42	1.37
24	y	312	CHL	CHD-C4C	3.46	1.47	1.39
24	r	309	CHL	CHD-C4C	3.46	1.47	1.39
24	g	311	CHL	C1D-ND	-3.46	1.33	1.37
24	R	607	CHL	CHC-C4B	3.46	1.47	1.39
24	5	310	CHL	C1D-ND	-3.46	1.33	1.37
25	q	306	CLA	C1D-ND	3.46	1.42	1.37
24	s	408	CHL	CHD-C4C	3.46	1.47	1.39
24	4	312	CHL	CHB-C1B	3.46	1.47	1.39
24	g	309	CHL	C1D-ND	-3.46	1.33	1.37
25	C	611	CLA	C1D-ND	3.46	1.42	1.37
24	N	309	CHL	CHD-C4C	3.46	1.47	1.39
24	r	308	CHL	CHC-C4B	3.46	1.47	1.39
24	y	312	CHL	OBD-CAD	3.46	1.28	1.22
24	s	409	CHL	C1D-ND	-3.46	1.33	1.37
24	n	309	CHL	CHD-C4C	3.46	1.47	1.39
24	N	308	CHL	CHB-C1B	3.46	1.47	1.39
24	N	310	CHL	CHB-C1B	3.46	1.47	1.39
24	n	304	CHL	CHB-C1B	3.46	1.47	1.39
24	g	318	CHL	C1D-ND	-3.46	1.33	1.37
24	y	305	CHL	CHC-C4B	3.46	1.47	1.39
24	R	606	CHL	CHD-C4C	3.46	1.47	1.39
24	8	310	CHL	OBD-CAD	3.45	1.28	1.22
24	p	318	CHL	C1D-ND	-3.45	1.33	1.37
25	B	609	CLA	C1D-ND	3.45	1.42	1.37
25	c	611	CLA	C1D-ND	3.45	1.42	1.37
24	y	306	CHL	CHC-C4B	3.45	1.47	1.39
24	r	303	CHL	CHD-C4C	3.45	1.47	1.39
24	Y	304	CHL	CHC-C4B	3.45	1.47	1.39
25	Y	307	CLA	C1D-ND	3.45	1.42	1.37
25	c	606	CLA	C4D-ND	-3.45	1.32	1.37
24	6	310	CHL	C3D-C2D	3.45	1.48	1.39
24	Y	311	CHL	CHD-C4C	3.45	1.47	1.39
24	q	310	CHL	OBD-CAD	3.45	1.28	1.22
24	N	305	CHL	CHD-C4C	3.45	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	308	CHL	OBD-CAD	3.45	1.28	1.22
24	q	309	CHL	CHD-C4C	3.45	1.47	1.39
24	Y	311	CHL	C1D-ND	-3.45	1.33	1.37
24	y	311	CHL	C1D-ND	-3.45	1.33	1.37
25	Y	315	CLA	C4D-ND	-3.45	1.33	1.37
24	Y	317	CHL	OBD-CAD	3.45	1.28	1.22
25	y	307	CLA	C1D-ND	3.45	1.42	1.37
25	q	312	CLA	C1D-ND	3.45	1.42	1.37
25	c	610	CLA	C4D-ND	-3.45	1.33	1.37
25	Y	306	CLA	C1D-ND	3.45	1.42	1.37
31	t	101	8CT	C11-C12	3.45	1.53	1.45
25	s	405	CLA	C1D-ND	3.45	1.42	1.37
24	q	311	CHL	OBD-CAD	3.45	1.28	1.22
31	v	401	8CT	C11-C12	3.45	1.53	1.45
25	S	616	CLA	C1D-ND	3.45	1.42	1.37
24	5	306	CHL	CHD-C4C	3.45	1.47	1.39
24	r	308	CHL	CHD-C4C	3.45	1.47	1.39
24	G	311	CHL	CHB-C1B	3.44	1.47	1.39
25	B	608	CLA	C1D-ND	3.44	1.42	1.37
24	7	312	CHL	OBD-CAD	3.44	1.28	1.22
26	q	302	0IE	C15-C16	3.44	1.40	1.35
24	p	310	CHL	CHB-C1B	3.44	1.47	1.39
24	7	309	CHL	C1D-ND	-3.44	1.33	1.37
25	8	306	CLA	C1D-ND	3.44	1.42	1.37
24	4	304	CHL	C3D-C2D	3.44	1.48	1.39
24	9	304	CHL	CHB-C1B	3.44	1.47	1.39
24	y	311	CHL	CHD-C4C	3.44	1.47	1.39
24	1	304	CHL	C1D-ND	-3.44	1.33	1.37
24	9	308	CHL	C1D-ND	-3.44	1.33	1.37
24	s	408	CHL	OBD-CAD	3.44	1.28	1.22
24	1	304	CHL	C3D-C2D	3.44	1.48	1.39
25	C	606	CLA	C4D-ND	-3.44	1.33	1.37
24	q	303	CHL	CHB-C1B	3.44	1.47	1.39
24	3	312	CHL	C3D-C2D	3.44	1.48	1.39
24	u	313	CHL	C3D-C2D	3.44	1.48	1.39
24	R	602	CHL	CHD-C4C	3.44	1.47	1.39
25	b	610	CLA	C4D-ND	-3.44	1.33	1.37
24	8	303	CHL	CHB-C1B	3.44	1.47	1.39
24	9	310	CHL	C3D-C2D	3.44	1.48	1.39
24	r	302	CHL	CHB-C1B	3.44	1.47	1.39
24	R	608	CHL	CHD-C4C	3.44	1.47	1.39
24	Y	311	CHL	OBD-CAD	3.44	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	u	318	CHL	C1D-ND	-3.43	1.33	1.37
25	b	607	CLA	C1D-ND	3.43	1.42	1.37
24	Y	305	CHL	CHC-C4B	3.43	1.47	1.39
24	6	317	CHL	C1D-ND	-3.43	1.33	1.37
31	V	401	8CT	C11-C12	3.43	1.53	1.45
31	a	608	8CT	C11-C12	3.43	1.53	1.45
25	C	607	CLA	C4D-ND	-3.43	1.33	1.37
24	y	318	CHL	OBD-CAD	3.43	1.28	1.22
24	4	304	CHL	C1D-ND	-3.43	1.33	1.37
24	u	311	CHL	C3D-C2D	3.43	1.48	1.39
25	a	605	CLA	C4D-ND	-3.43	1.33	1.37
24	G	318	CHL	C1D-ND	-3.43	1.33	1.37
24	7	305	CHL	CHC-C4B	3.43	1.47	1.39
24	5	312	CHL	C1D-ND	-3.43	1.33	1.37
24	u	311	CHL	C1D-ND	-3.43	1.33	1.37
24	R	607	CHL	CHD-C4C	3.43	1.47	1.39
24	g	309	CHL	C3D-C2D	3.43	1.48	1.39
24	1	308	CHL	C1D-ND	-3.43	1.33	1.37
24	9	317	CHL	C3D-C2D	3.43	1.48	1.39
31	T	101	8CT	C11-C12	3.43	1.53	1.45
25	C	602	CLA	C4D-ND	-3.43	1.33	1.37
24	2	306	CHL	CHD-C4C	3.43	1.47	1.39
24	n	311	CHL	CHD-C4C	3.43	1.47	1.39
24	N	312	CHL	C1D-ND	-3.43	1.33	1.37
24	p	305	CHL	C1D-ND	-3.43	1.33	1.37
31	d	410	8CT	C01-C02	3.43	1.56	1.50
24	3	305	CHL	CHB-C1B	3.43	1.47	1.39
24	G	310	CHL	C1D-ND	-3.43	1.33	1.37
25	B	613	CLA	C4D-ND	-3.42	1.33	1.37
24	9	308	CHL	C3D-C2D	3.42	1.48	1.39
24	g	310	CHL	C1D-ND	-3.42	1.33	1.37
25	c	604	CLA	C4D-ND	-3.42	1.33	1.37
24	1	317	CHL	C3D-C2D	3.42	1.48	1.39
24	5	310	CHL	CHD-C4C	3.42	1.47	1.39
25	8	305	CLA	C1D-ND	3.42	1.42	1.37
24	6	312	CHL	C3D-C2D	3.42	1.48	1.39
24	3	310	CHL	C3D-C2D	3.42	1.48	1.39
24	G	309	CHL	C3D-C2D	3.42	1.48	1.39
24	u	309	CHL	C3D-C2D	3.42	1.48	1.39
25	q	305	CLA	C1D-ND	3.42	1.42	1.37
24	u	318	CHL	C3D-C2D	3.42	1.48	1.39
24	N	305	CHL	CHB-C1B	3.42	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	306	CHL	C3A-C2A	-3.42	1.51	1.54
24	r	307	CHL	CHD-C4C	3.42	1.47	1.39
24	1	309	CHL	C1D-ND	-3.42	1.33	1.37
25	B	616	CLA	C1D-ND	3.42	1.42	1.37
25	p	307	CLA	C1D-ND	3.42	1.42	1.37
28	7	304	NEX	C7-C8	-3.42	1.26	1.32
25	C	616	CLA	C4D-ND	-3.42	1.33	1.37
24	3	308	CHL	C3D-C2D	3.42	1.48	1.39
24	9	312	CHL	C3D-C2D	3.42	1.48	1.39
24	n	309	CHL	C1D-ND	-3.41	1.33	1.37
24	r	306	CHL	CHB-C1B	3.41	1.47	1.39
25	y	308	CLA	C1D-ND	3.41	1.42	1.37
24	3	308	CHL	C1D-ND	-3.41	1.33	1.37
24	9	310	CHL	C1D-ND	-3.41	1.33	1.37
24	u	306	CHL	CHB-C1B	3.41	1.47	1.39
28	r	317	NEX	C7-C8	-3.41	1.26	1.32
24	S	613	CHL	CHD-C4C	3.41	1.47	1.39
25	c	616	CLA	C4D-ND	-3.41	1.33	1.37
24	n	310	CHL	CHB-C1B	3.41	1.47	1.39
24	7	305	CHL	C1D-ND	-3.41	1.33	1.37
25	b	616	CLA	C1D-ND	3.41	1.42	1.37
25	s	412	CLA	C1D-ND	3.41	1.42	1.37
24	4	308	CHL	C3D-C2D	3.41	1.48	1.39
25	y	315	CLA	C4D-ND	-3.41	1.33	1.37
24	7	305	CHL	CHD-C4C	3.41	1.47	1.39
24	N	309	CHL	C1D-ND	-3.41	1.33	1.37
24	G	309	CHL	C1D-ND	-3.41	1.33	1.37
24	s	414	CHL	CHD-C4C	3.41	1.47	1.39
24	p	311	CHL	CHB-C1B	3.41	1.47	1.39
24	6	309	CHL	C1D-ND	-3.40	1.33	1.37
24	S	601	CHL	CHD-C4C	3.40	1.47	1.39
25	a	607	CLA	C1D-ND	3.40	1.42	1.37
24	6	308	CHL	C3D-C2D	3.40	1.48	1.39
24	g	313	CHL	C3D-C2D	3.40	1.48	1.39
25	9	316	CLA	C4B-NB	3.40	1.42	1.37
25	b	608	CLA	C1D-ND	3.40	1.42	1.37
24	4	310	CHL	CHB-C1B	3.40	1.47	1.39
24	r	302	CHL	C3D-C2D	3.40	1.48	1.39
24	p	305	CHL	CHD-C4C	3.40	1.47	1.39
24	R	601	CHL	CHB-C1B	3.40	1.47	1.39
24	2	310	CHL	CHB-C1B	3.40	1.47	1.39
24	N	304	CHL	C1D-ND	-3.40	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	303	CHL	C3D-C2D	3.40	1.48	1.39
24	q	316	CHL	C3A-C2A	-3.40	1.51	1.54
26	y	303	0IE	C15-C16	3.40	1.40	1.35
24	g	310	CHL	C3D-C2D	3.40	1.48	1.39
25	Y	314	CLA	C4D-ND	-3.40	1.33	1.37
24	2	305	CHL	C1D-ND	-3.40	1.33	1.37
24	u	305	CHL	C1D-ND	-3.40	1.33	1.37
25	S	610	CLA	C1D-ND	3.40	1.42	1.37
25	8	311	CLA	C1D-ND	3.40	1.42	1.37
24	8	304	CHL	CHD-C4C	3.40	1.47	1.39
24	6	308	CHL	C1D-ND	-3.40	1.33	1.37
24	6	312	CHL	C1D-ND	-3.40	1.33	1.37
24	n	311	CHL	C1D-ND	-3.40	1.33	1.37
25	u	317	CLA	C4B-NB	3.40	1.42	1.37
24	q	304	CHL	CHD-C4C	3.39	1.47	1.39
24	G	313	CHL	C3D-C2D	3.39	1.48	1.39
24	g	311	CHL	C3D-C2D	3.39	1.48	1.39
24	6	304	CHL	C1D-ND	-3.39	1.33	1.37
24	4	317	CHL	C3D-C2D	3.39	1.48	1.39
24	4	305	CHL	C1D-ND	-3.39	1.33	1.37
25	S	612	CLA	C1D-ND	3.39	1.42	1.37
24	n	317	CHL	C3D-C2D	3.39	1.48	1.39
24	N	304	CHL	C3D-C2D	3.39	1.48	1.39
24	G	313	CHL	C1D-ND	-3.39	1.33	1.37
24	q	308	CHL	CHD-C4C	3.39	1.47	1.39
24	R	605	CHL	CHD-C4C	3.39	1.47	1.39
24	5	305	CHL	C1D-ND	-3.39	1.33	1.37
24	7	318	CHL	CHB-C1B	3.39	1.47	1.39
24	8	308	CHL	CHD-C4C	3.39	1.47	1.39
24	6	309	CHL	C3D-C2D	3.39	1.48	1.39
25	d	405	CLA	C4D-ND	-3.39	1.33	1.37
24	4	311	CHL	C1D-ND	-3.39	1.33	1.37
24	g	306	CHL	C1D-ND	-3.39	1.33	1.37
25	d	405	CLA	C1D-ND	3.39	1.41	1.37
25	B	603	CLA	C4D-ND	-3.39	1.33	1.37
25	A	605	CLA	C4D-ND	-3.39	1.33	1.37
25	D	405	CLA	C4D-ND	-3.39	1.33	1.37
24	G	306	CHL	C1D-ND	-3.39	1.33	1.37
24	N	317	CHL	C3D-C2D	3.38	1.48	1.39
25	b	609	CLA	C1D-ND	3.38	1.41	1.37
31	A	608	8CT	C11-C12	3.38	1.53	1.45
24	n	312	CHL	CHB-C1B	3.38	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	C4D-ND	-3.38	1.33	1.37
24	Y	317	CHL	CHD-C4C	3.38	1.47	1.39
25	R	612	CLA	C4B-NB	3.38	1.41	1.37
24	1	308	CHL	C3D-C2D	3.38	1.48	1.39
24	1	310	CHL	CHB-C1B	3.38	1.47	1.39
25	b	603	CLA	C4D-ND	-3.38	1.33	1.37
24	8	315	CHL	C3D-C2D	3.38	1.48	1.39
24	4	317	CHL	C1D-ND	-3.38	1.33	1.37
24	n	305	CHL	CHB-C1B	3.38	1.47	1.39
28	y	304	NEX	C7-C8	-3.38	1.26	1.32
24	9	305	CHL	CHB-C1B	3.38	1.47	1.39
24	7	312	CHL	C1D-ND	-3.38	1.33	1.37
25	9	314	CLA	C4B-NB	3.38	1.41	1.37
25	Y	313	CLA	C1D-ND	3.38	1.41	1.37
24	N	311	CHL	C1D-ND	-3.38	1.33	1.37
25	B	613	CLA	C1D-ND	3.38	1.41	1.37
24	p	305	CHL	CHC-C4B	3.38	1.47	1.39
24	3	309	CHL	C3D-C2D	3.38	1.48	1.39
24	9	317	CHL	C1D-ND	-3.37	1.33	1.37
28	G	304	NEX	C7-C8	-3.37	1.26	1.32
25	C	601	CLA	C1D-ND	3.37	1.41	1.37
28	1	303	NEX	C7-C8	-3.37	1.26	1.32
25	s	411	CLA	C1D-ND	3.37	1.41	1.37
24	G	310	CHL	C3D-C2D	3.37	1.48	1.39
24	4	312	CHL	C3D-C2D	3.37	1.48	1.39
24	6	305	CHL	CHB-C1B	3.37	1.47	1.39
24	R	608	CHL	CHB-C1B	3.37	1.47	1.39
24	3	311	CHL	CHB-C1B	3.37	1.47	1.39
28	g	304	NEX	C7-C8	-3.37	1.26	1.32
24	R	601	CHL	C3D-C2D	3.37	1.48	1.39
24	1	311	CHL	C1D-ND	-3.37	1.33	1.37
24	n	304	CHL	C3D-C2D	3.37	1.48	1.39
24	p	306	CHL	OBD-CAD	3.37	1.28	1.22
24	g	313	CHL	C1D-ND	-3.37	1.33	1.37
28	R	616	NEX	C7-C8	-3.37	1.26	1.32
28	4	303	NEX	C7-C8	-3.37	1.26	1.32
25	C	611	CLA	C4D-ND	-3.37	1.33	1.37
25	1	315	CLA	C4B-NB	3.37	1.41	1.37
25	y	317	CLA	C1D-ND	3.37	1.41	1.37
25	b	613	CLA	C4D-ND	-3.37	1.33	1.37
24	N	312	CHL	CHB-C1B	3.37	1.47	1.39
24	S	608	CHL	C1D-ND	-3.37	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	309	CHL	CHD-C4C	3.36	1.46	1.39
24	p	318	CHL	CHB-C1B	3.36	1.47	1.39
25	A	603	CLA	C1D-ND	3.36	1.41	1.37
35	D	403	PHO	C1D-C2D	3.36	1.43	1.39
24	2	311	CHL	C3D-C2D	3.36	1.48	1.39
24	y	318	CHL	CHD-C4C	3.36	1.46	1.39
24	n	304	CHL	C1D-ND	-3.36	1.33	1.37
25	a	610	CLA	C4B-NB	3.36	1.41	1.37
24	3	309	CHL	C1D-ND	-3.36	1.33	1.37
24	p	309	CHL	C1D-ND	-3.36	1.33	1.37
24	q	316	CHL	C3D-C2D	3.36	1.48	1.39
24	q	310	CHL	CHD-C4C	3.36	1.46	1.39
24	S	608	CHL	CHB-C1B	3.36	1.46	1.39
25	B	615	CLA	C1D-ND	3.36	1.41	1.37
25	C	604	CLA	C4D-ND	-3.36	1.33	1.37
24	q	307	CHL	CHB-C1B	3.36	1.46	1.39
24	9	317	CHL	C3A-C2A	-3.36	1.51	1.54
24	5	311	CHL	C3D-C2D	3.36	1.48	1.39
24	q	303	CHL	C3D-C2D	3.36	1.48	1.39
24	G	311	CHL	C3D-C2D	3.36	1.48	1.39
24	1	312	CHL	C3D-C2D	3.36	1.48	1.39
24	u	306	CHL	C3D-C2D	3.36	1.48	1.39
25	A	607	CLA	C1D-ND	3.36	1.41	1.37
25	B	612	CLA	C4D-ND	-3.35	1.33	1.37
24	2	312	CHL	C1D-ND	-3.35	1.33	1.37
24	7	311	CHL	CHB-C1B	3.35	1.46	1.39
24	N	310	CHL	C3D-C2D	3.35	1.48	1.39
24	5	309	CHL	MG-NA	-3.35	1.98	2.06
24	5	318	CHL	C3D-C2D	3.35	1.48	1.39
24	G	306	CHL	CHB-C1B	3.35	1.46	1.39
24	r	308	CHL	C1D-ND	-3.35	1.33	1.37
24	s	409	CHL	CHB-C1B	3.35	1.46	1.39
24	7	306	CHL	OBD-CAD	3.35	1.28	1.22
24	5	310	CHL	CHB-C1B	3.35	1.46	1.39
24	Y	310	CHL	CHD-C4C	3.35	1.46	1.39
24	9	304	CHL	C3D-C2D	3.35	1.48	1.39
24	n	308	CHL	C3D-C2D	3.35	1.48	1.39
25	b	605	CLA	C1D-ND	3.35	1.41	1.37
24	u	309	CHL	C1D-ND	-3.35	1.33	1.37
24	n	312	CHL	C1D-ND	-3.35	1.33	1.37
24	s	406	CHL	CHB-C1B	3.35	1.46	1.39
24	N	305	CHL	C3D-C2D	3.35	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	316	CHL	C1D-ND	-3.34	1.33	1.37
25	1	316	CLA	C4B-NB	3.34	1.41	1.37
26	Y	303	0IE	C15-C16	3.34	1.40	1.35
24	1	305	CHL	C1D-ND	-3.34	1.33	1.37
25	b	608	CLA	C4D-ND	-3.34	1.33	1.37
35	d	403	PHO	C1D-C2D	3.34	1.43	1.39
24	R	607	CHL	C1D-ND	-3.34	1.33	1.37
25	b	614	CLA	C4D-ND	-3.34	1.33	1.37
24	Y	304	CHL	CHD-C4C	3.34	1.46	1.39
25	4	314	CLA	C4B-NB	3.34	1.41	1.37
24	n	317	CHL	C1D-ND	-3.34	1.33	1.37
24	u	305	CHL	C3D-C2D	3.34	1.48	1.39
24	G	312	CHL	C3D-C2D	3.34	1.48	1.39
25	S	611	CLA	C1D-ND	3.34	1.41	1.37
24	Y	312	CHL	OBD-CAD	3.34	1.28	1.22
25	C	608	CLA	C4D-ND	-3.34	1.33	1.37
25	1	314	CLA	C4B-NB	3.34	1.41	1.37
24	8	315	CHL	C3A-C2A	-3.34	1.51	1.54
24	3	312	CHL	C1D-ND	-3.34	1.33	1.37
24	N	308	CHL	C3D-C2D	3.34	1.48	1.39
25	S	612	CLA	C4D-ND	-3.34	1.33	1.37
24	2	318	CHL	C3D-C2D	3.34	1.48	1.39
24	n	312	CHL	C3D-C2D	3.34	1.48	1.39
23	f	201	HEM	FE-ND	3.34	2.05	1.94
25	b	602	CLA	C1D-ND	3.33	1.41	1.37
24	g	312	CHL	C3D-C2D	3.33	1.48	1.39
24	n	310	CHL	C3D-C2D	3.33	1.48	1.39
25	B	614	CLA	C4D-ND	-3.33	1.33	1.37
25	C	601	CLA	C4D-ND	-3.33	1.33	1.37
24	G	309	CHL	MG-NA	-3.33	1.98	2.06
25	Y	316	CLA	C1D-ND	3.33	1.41	1.37
24	1	310	CHL	C3D-C2D	3.33	1.48	1.39
24	5	309	CHL	C3D-C2D	3.33	1.48	1.39
24	u	310	CHL	C3D-C2D	3.33	1.48	1.39
24	G	305	CHL	CHB-C1B	3.33	1.46	1.39
24	4	309	CHL	C3D-C2D	3.33	1.48	1.39
24	S	605	CHL	CHB-C1B	3.33	1.46	1.39
25	c	608	CLA	C4D-ND	-3.33	1.33	1.37
24	g	318	CHL	CHB-C1B	3.33	1.46	1.39
25	D	405	CLA	C1D-ND	3.33	1.41	1.37
25	B	602	CLA	C4D-ND	-3.33	1.33	1.37
24	1	304	CHL	MG-NA	-3.33	1.98	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	310	CHL	C3D-C2D	3.33	1.48	1.39
24	4	311	CHL	CHB-C1B	3.33	1.46	1.39
25	a	607	CLA	C4D-ND	-3.33	1.33	1.37
24	1	309	CHL	C3D-C2D	3.33	1.48	1.39
25	B	605	CLA	C4D-ND	-3.32	1.33	1.37
24	4	304	CHL	MG-NA	-3.32	1.98	2.06
24	n	305	CHL	C3D-C2D	3.32	1.48	1.39
24	7	313	CHL	CHB-C1B	3.32	1.46	1.39
25	C	612	CLA	C4D-ND	-3.32	1.33	1.37
25	S	610	CLA	C4D-ND	-3.32	1.33	1.37
25	u	315	CLA	C4B-NB	3.32	1.41	1.37
24	r	309	CHL	CHB-C1B	3.32	1.46	1.39
25	y	314	CLA	C1D-ND	3.32	1.41	1.37
24	1	317	CHL	C1D-ND	-3.32	1.33	1.37
28	u	304	NEX	C7-C8	-3.31	1.26	1.32
24	3	305	CHL	C3D-C2D	3.31	1.48	1.39
25	4	316	CLA	C4B-NB	3.31	1.41	1.37
25	b	613	CLA	C1D-ND	3.31	1.41	1.37
24	9	305	CHL	C3D-C2D	3.31	1.48	1.39
24	5	305	CHL	CHB-C1B	3.31	1.46	1.39
25	b	611	CLA	C4D-ND	-3.31	1.33	1.37
24	9	309	CHL	C3D-C2D	3.31	1.48	1.39
24	p	318	CHL	C3D-C2D	3.31	1.48	1.39
24	r	306	CHL	C3D-C2D	3.31	1.48	1.39
28	p	304	NEX	C7-C8	-3.31	1.26	1.32
28	2	304	NEX	C7-C8	-3.31	1.26	1.32
24	p	312	CHL	CHD-C4C	3.31	1.46	1.39
24	9	304	CHL	C1D-ND	-3.31	1.33	1.37
24	7	318	CHL	C3D-C2D	3.31	1.48	1.39
24	S	606	CHL	CHB-C1B	3.31	1.46	1.39
24	p	313	CHL	CHB-C1B	3.31	1.46	1.39
24	N	312	CHL	C3D-C2D	3.31	1.48	1.39
25	Y	316	CLA	C4D-ND	-3.31	1.33	1.37
25	G	307	CLA	C4B-NB	3.31	1.41	1.37
24	u	312	CHL	C1D-ND	-3.31	1.33	1.37
24	g	305	CHL	CHB-C1B	3.31	1.46	1.39
25	s	411	CLA	C4D-ND	-3.31	1.33	1.37
31	c	614	8CT	C07-C02	-3.31	1.44	1.51
25	b	612	CLA	C4D-ND	-3.31	1.33	1.37
25	u	307	CLA	C4B-NB	3.31	1.41	1.37
24	R	605	CHL	C1D-ND	-3.31	1.33	1.37
25	c	608	CLA	C1D-ND	3.31	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	608	8CT	C28-C29	3.31	1.40	1.32
25	c	612	CLA	C4D-ND	-3.31	1.33	1.37
24	6	311	CHL	CHB-C1B	3.31	1.46	1.39
24	N	317	CHL	C1D-ND	-3.30	1.33	1.37
24	7	309	CHL	MG-NA	-3.30	1.98	2.06
24	6	304	CHL	CHB-C1B	3.30	1.46	1.39
25	A	610	CLA	C4B-NB	3.30	1.41	1.37
24	2	309	CHL	C3D-C2D	3.30	1.48	1.39
25	B	608	CLA	C4D-ND	-3.30	1.33	1.37
25	b	615	CLA	C4D-ND	-3.30	1.33	1.37
25	C	603	CLA	C4D-ND	-3.30	1.33	1.37
25	c	603	CLA	C4D-ND	-3.30	1.33	1.37
24	9	311	CHL	C1D-ND	-3.30	1.33	1.37
25	a	603	CLA	C1D-ND	3.30	1.41	1.37
25	s	413	CLA	C1D-ND	3.30	1.41	1.37
25	b	615	CLA	C1D-ND	3.30	1.41	1.37
25	c	601	CLA	C1D-ND	3.30	1.41	1.37
25	y	316	CLA	C1D-ND	3.30	1.41	1.37
24	u	318	CHL	C3A-C2A	-3.30	1.51	1.54
24	4	308	CHL	MG-NA	-3.30	1.98	2.06
31	C	613	8CT	C28-C29	3.30	1.40	1.32
25	c	609	CLA	C1D-ND	3.30	1.41	1.37
25	Y	314	CLA	C1D-ND	3.30	1.41	1.37
25	c	602	CLA	C1D-ND	3.30	1.41	1.37
25	B	615	CLA	C4D-ND	-3.30	1.33	1.37
24	Y	308	CHL	CHB-C1B	3.30	1.46	1.39
24	G	312	CHL	C1D-ND	-3.30	1.33	1.37
24	g	309	CHL	MG-NA	-3.29	1.98	2.06
25	B	611	CLA	C4D-ND	-3.29	1.33	1.37
24	3	304	CHL	C1D-ND	-3.29	1.33	1.37
24	s	403	CHL	CHB-C1B	3.29	1.46	1.39
25	c	611	CLA	C4D-ND	-3.29	1.33	1.37
24	8	315	CHL	C1D-ND	-3.29	1.33	1.37
25	C	608	CLA	C1D-ND	3.29	1.41	1.37
24	8	307	CHL	CHB-C1B	3.29	1.46	1.39
25	b	612	CLA	C1D-ND	3.29	1.41	1.37
24	G	318	CHL	CHB-C1B	3.29	1.46	1.39
24	1	308	CHL	MG-NA	-3.29	1.98	2.06
24	6	304	CHL	C3D-C2D	3.29	1.48	1.39
24	2	305	CHL	CHB-C1B	3.29	1.46	1.39
25	B	605	CLA	C1D-ND	3.29	1.41	1.37
24	p	310	CHL	C3D-C2D	3.29	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	310	CHL	C3D-C2D	3.29	1.48	1.39
28	S	617	NEX	C7-C8	-3.29	1.26	1.32
24	S	607	CHL	C1D-ND	-3.29	1.33	1.37
25	C	603	CLA	C1D-ND	3.29	1.41	1.37
25	a	605	CLA	C1D-ND	3.29	1.41	1.37
25	c	606	CLA	C1D-ND	3.29	1.41	1.37
24	5	318	CHL	MG-NA	-3.29	1.98	2.06
24	S	602	CHL	CHB-C1B	3.29	1.46	1.39
24	g	305	CHL	C3D-C2D	3.29	1.48	1.39
35	a	606	PHO	C1D-C2D	3.28	1.43	1.39
24	4	317	CHL	MG-NA	-3.28	1.98	2.06
25	s	413	CLA	C4D-ND	-3.28	1.33	1.37
31	C	614	8CT	C28-C29	3.28	1.40	1.32
24	y	310	CHL	CHD-C4C	3.28	1.46	1.39
25	y	307	CLA	C4D-ND	-3.28	1.33	1.37
25	3	316	CLA	C4B-NB	3.28	1.41	1.37
28	5	304	NEX	C7-C8	-3.28	1.26	1.32
24	6	317	CHL	C3D-C2D	3.28	1.48	1.39
24	u	318	CHL	MG-NA	-3.28	1.98	2.06
25	u	314	CLA	C4B-NB	3.28	1.41	1.37
25	b	602	CLA	C4D-ND	-3.28	1.33	1.37
25	9	315	CLA	C4B-NB	3.28	1.41	1.37
25	Y	315	CLA	C1D-ND	3.28	1.41	1.37
24	y	309	CHL	CHB-C1B	3.28	1.46	1.39
31	c	614	8CT	C28-C29	3.28	1.40	1.32
24	3	304	CHL	CHB-C1B	3.28	1.46	1.39
25	6	307	CLA	C4B-NB	3.28	1.41	1.37
31	X	601	8CT	C28-C29	3.28	1.40	1.32
24	Y	309	CHL	CHD-C4C	3.28	1.46	1.39
24	G	305	CHL	C3D-C2D	3.28	1.48	1.39
31	c	613	8CT	C28-C29	3.27	1.40	1.32
24	2	318	CHL	MG-NA	-3.27	1.98	2.06
25	B	616	CLA	C4D-ND	-3.27	1.33	1.37
25	B	602	CLA	C1D-ND	3.27	1.41	1.37
24	2	313	CHL	C3D-C2D	3.27	1.48	1.39
24	n	317	CHL	MG-NA	-3.27	1.98	2.06
24	N	317	CHL	MG-NA	-3.27	1.98	2.06
24	1	305	CHL	CHB-C1B	3.27	1.46	1.39
24	y	305	CHL	CHD-C4C	3.27	1.46	1.39
24	8	303	CHL	MG-NA	-3.27	1.98	2.06
31	A	608	8CT	C01-C02	3.27	1.56	1.50
25	n	306	CLA	C4B-NB	3.27	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	305	CHL	C3D-C2D	3.27	1.48	1.39
24	5	305	CHL	C3D-C2D	3.27	1.48	1.39
28	9	319	NEX	C7-C8	-3.27	1.26	1.32
31	x	601	8CT	C28-C29	3.27	1.40	1.32
25	s	405	CLA	C4D-ND	-3.27	1.33	1.37
25	Y	313	CLA	C4D-ND	-3.27	1.33	1.37
35	A	606	PHO	C1D-C2D	3.27	1.43	1.39
25	n	314	CLA	C4B-NB	3.27	1.41	1.37
24	7	311	CHL	C3D-C2D	3.27	1.48	1.39
24	3	317	CHL	C3D-C2D	3.27	1.48	1.39
24	5	313	CHL	C3D-C2D	3.27	1.48	1.39
25	3	313	CLA	C4B-NB	3.27	1.41	1.37
25	7	317	CLA	C4B-NB	3.27	1.41	1.37
24	9	311	CHL	C3D-C2D	3.26	1.48	1.39
24	R	602	CHL	CHB-C1B	3.26	1.46	1.39
24	g	306	CHL	CHB-C1B	3.26	1.46	1.39
24	3	311	CHL	C1D-ND	-3.26	1.33	1.37
25	y	314	CLA	C4D-ND	-3.26	1.33	1.37
24	6	311	CHL	C1D-ND	-3.26	1.33	1.37
25	b	614	CLA	C1D-ND	3.26	1.41	1.37
24	u	312	CHL	C3D-C2D	3.26	1.48	1.39
25	6	316	CLA	C4B-NB	3.26	1.41	1.37
25	c	612	CLA	C1D-ND	3.26	1.41	1.37
24	r	307	CHL	CHB-C1B	3.26	1.46	1.39
24	9	317	CHL	MG-NA	-3.26	1.98	2.06
24	p	306	CHL	CHD-C4C	3.26	1.46	1.39
24	p	311	CHL	C3D-C2D	3.26	1.48	1.39
25	A	607	CLA	C4D-ND	-3.26	1.33	1.37
25	6	315	CLA	C4B-NB	3.26	1.41	1.37
24	y	313	CHL	CHB-C1B	3.26	1.46	1.39
24	s	407	CHL	CHB-C1B	3.26	1.46	1.39
24	p	309	CHL	MG-NA	-3.26	1.98	2.06
25	B	609	CLA	C4D-ND	-3.26	1.33	1.37
31	a	608	8CT	C28-C29	3.26	1.40	1.32
25	g	307	CLA	C4B-NB	3.26	1.41	1.37
24	7	306	CHL	CHD-C4C	3.26	1.46	1.39
24	6	305	CHL	C3D-C2D	3.26	1.48	1.39
25	q	306	CLA	C4D-ND	-3.25	1.33	1.37
23	E	201	HEM	FE-ND	3.25	2.04	1.94
24	q	309	CHL	CHB-C1B	3.25	1.46	1.39
25	C	606	CLA	C1D-ND	3.25	1.41	1.37
25	n	307	CLA	C4B-NB	3.25	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	312	CHL	C1D-ND	-3.25	1.33	1.37
24	R	606	CHL	CHB-C1B	3.25	1.46	1.39
25	9	313	CLA	C4B-NB	3.25	1.41	1.37
24	G	318	CHL	C3D-C2D	3.25	1.48	1.39
24	7	312	CHL	CHD-C4C	3.25	1.46	1.39
24	4	305	CHL	CHB-C1B	3.25	1.46	1.39
24	1	311	CHL	CHB-C1B	3.25	1.46	1.39
25	8	306	CLA	C4D-ND	-3.25	1.33	1.37
25	9	307	CLA	C4B-NB	3.25	1.41	1.37
25	N	307	CLA	C4B-NB	3.24	1.41	1.37
25	C	604	CLA	C1D-ND	3.24	1.41	1.37
24	q	307	CHL	C3D-C2D	3.24	1.48	1.39
24	u	305	CHL	MG-NA	-3.24	1.98	2.06
25	Y	307	CLA	C4D-ND	-3.24	1.33	1.37
25	4	315	CLA	C4B-NB	3.24	1.41	1.37
24	9	308	CHL	MG-NA	-3.24	1.98	2.06
24	3	304	CHL	C3D-C2D	3.24	1.48	1.39
25	y	315	CLA	C1D-ND	3.24	1.41	1.37
25	Y	306	CLA	C4D-ND	-3.24	1.33	1.37
25	b	616	CLA	C4D-ND	-3.24	1.33	1.37
31	a	608	8CT	C01-C02	3.24	1.56	1.50
24	s	406	CHL	C3D-C2D	3.24	1.48	1.39
24	8	307	CHL	C3D-C2D	3.24	1.48	1.39
25	C	605	CLA	C4D-ND	-3.24	1.33	1.37
24	N	311	CHL	CHB-C1B	3.24	1.46	1.39
24	r	309	CHL	C3D-C2D	3.23	1.48	1.39
25	c	603	CLA	C1D-ND	3.23	1.41	1.37
31	s	415	8CT	C01-C02	3.23	1.56	1.50
24	1	317	CHL	MG-NA	-3.23	1.98	2.06
24	5	312	CHL	CHB-C1B	3.23	1.46	1.39
25	u	308	CLA	C4B-NB	3.23	1.41	1.37
24	q	303	CHL	MG-NA	-3.23	1.98	2.06
25	b	609	CLA	C4D-ND	-3.23	1.33	1.37
25	S	603	CLA	C4D-ND	-3.23	1.33	1.37
25	c	605	CLA	C4D-ND	-3.23	1.33	1.37
25	s	412	CLA	C4D-ND	-3.23	1.33	1.37
25	7	316	CLA	C4D-ND	-3.23	1.33	1.37
24	g	318	CHL	C3D-C2D	3.23	1.47	1.39
24	s	409	CHL	C3D-C2D	3.23	1.47	1.39
24	s	408	CHL	C1D-ND	-3.23	1.33	1.37
25	C	609	CLA	C1D-ND	3.23	1.41	1.37
25	C	612	CLA	C1D-ND	3.23	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	313	CLA	C4B-NB	3.23	1.41	1.37
31	v	401	8CT	C01-C02	3.23	1.56	1.50
24	5	306	CHL	C3D-C2D	3.23	1.47	1.39
24	g	312	CHL	C1D-ND	-3.23	1.33	1.37
25	c	604	CLA	C1D-ND	3.23	1.41	1.37
24	r	303	CHL	CHB-C1B	3.23	1.46	1.39
24	9	312	CHL	MG-NA	-3.23	1.98	2.06
25	g	308	CLA	C4B-NB	3.23	1.41	1.37
25	S	611	CLA	C4D-ND	-3.23	1.33	1.37
24	R	608	CHL	C3D-C2D	3.23	1.47	1.39
24	n	311	CHL	CHB-C1B	3.23	1.46	1.39
25	b	604	CLA	C4D-ND	-3.23	1.33	1.37
24	2	312	CHL	CHB-C1B	3.23	1.46	1.39
24	S	606	CHL	C3D-C2D	3.23	1.47	1.39
24	5	310	CHL	C3D-C2D	3.23	1.47	1.39
24	p	312	CHL	CHB-C1B	3.22	1.46	1.39
24	2	309	CHL	MG-NA	-3.22	1.98	2.06
24	p	313	CHL	C3D-C2D	3.22	1.47	1.39
24	7	313	CHL	C3D-C2D	3.22	1.47	1.39
25	N	316	CLA	C4B-NB	3.22	1.41	1.37
24	s	407	CHL	C3D-C2D	3.22	1.47	1.39
25	c	601	CLA	C4D-ND	-3.22	1.33	1.37
24	G	306	CHL	C3D-C2D	3.22	1.47	1.39
25	3	314	CLA	C4B-NB	3.22	1.41	1.37
24	Y	312	CHL	CHB-C1B	3.22	1.46	1.39
25	n	316	CLA	C4B-NB	3.22	1.41	1.37
25	b	610	CLA	C1D-ND	3.22	1.41	1.37
25	G	316	CLA	C4B-NB	3.22	1.41	1.37
25	C	602	CLA	C1D-ND	3.22	1.41	1.37
25	u	316	CLA	C4B-NB	3.22	1.41	1.37
25	A	605	CLA	C1D-ND	3.22	1.41	1.37
25	r	313	CLA	C4B-NB	3.22	1.41	1.37
25	S	604	CLA	C4D-ND	-3.22	1.33	1.37
24	Y	305	CHL	CHD-C4C	3.22	1.46	1.39
24	2	310	CHL	C3D-C2D	3.22	1.47	1.39
31	C	614	8CT	C07-C02	-3.22	1.44	1.51
24	u	313	CHL	MG-NA	-3.21	1.98	2.06
25	9	306	CLA	C4B-NB	3.21	1.41	1.37
24	N	309	CHL	CHB-C1B	3.21	1.46	1.39
24	8	304	CHL	CHB-C1B	3.21	1.46	1.39
25	B	604	CLA	C4D-ND	-3.21	1.33	1.37
24	r	307	CHL	C3D-C2D	3.21	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	310	CHL	C3D-C2D	3.21	1.47	1.39
31	X	601	8CT	C01-C02	3.21	1.56	1.50
24	S	605	CHL	C3D-C2D	3.21	1.47	1.39
25	3	315	CLA	C4B-NB	3.21	1.41	1.37
25	p	317	CLA	C4B-NB	3.21	1.41	1.37
24	s	408	CHL	CHB-C1B	3.21	1.46	1.39
24	g	306	CHL	C3D-C2D	3.21	1.47	1.39
25	A	604	CLA	C1D-ND	3.20	1.41	1.37
25	y	317	CLA	C4D-ND	-3.20	1.33	1.37
24	7	312	CHL	CHB-C1B	3.20	1.46	1.39
25	b	603	CLA	C1D-ND	3.20	1.41	1.37
25	n	313	CLA	C4B-NB	3.20	1.41	1.37
25	B	612	CLA	C1D-ND	3.20	1.41	1.37
25	6	313	CLA	C4B-NB	3.20	1.41	1.37
25	s	417	CLA	C4D-ND	-3.20	1.33	1.37
25	B	607	CLA	C4D-ND	-3.20	1.33	1.37
25	y	308	CLA	C4D-ND	-3.20	1.33	1.37
25	B	610	CLA	C1D-ND	3.20	1.41	1.37
25	b	607	CLA	C4D-ND	-3.20	1.33	1.37
25	N	314	CLA	C4B-NB	3.20	1.41	1.37
24	8	308	CHL	CHB-C1B	3.20	1.46	1.39
24	y	306	CHL	CHD-C4C	3.20	1.46	1.39
25	c	607	CLA	C1D-ND	3.20	1.41	1.37
24	S	613	CHL	CHB-C1B	3.20	1.46	1.39
24	S	608	CHL	C3D-C2D	3.20	1.47	1.39
25	G	308	CLA	C4B-NB	3.20	1.41	1.37
25	B	614	CLA	C1D-ND	3.20	1.41	1.37
25	4	306	CLA	C4B-NB	3.20	1.41	1.37
25	a	604	CLA	C1D-ND	3.19	1.41	1.37
25	7	314	CLA	C4D-ND	-3.19	1.33	1.37
24	Y	308	CHL	C3D-C2D	3.19	1.47	1.39
24	2	306	CHL	CHB-C1B	3.19	1.46	1.39
31	c	615	8CT	C35-C30	3.19	1.65	1.56
25	1	313	CLA	C4B-NB	3.19	1.41	1.37
25	N	315	CLA	C4B-NB	3.19	1.41	1.37
25	B	611	CLA	C1D-ND	3.19	1.41	1.37
24	2	306	CHL	C3D-C2D	3.19	1.47	1.39
25	n	315	CLA	C4B-NB	3.19	1.41	1.37
24	y	309	CHL	C3D-C2D	3.19	1.47	1.39
24	q	310	CHL	CHB-C1B	3.19	1.46	1.39
24	R	601	CHL	MG-NA	-3.19	1.98	2.06
31	x	601	8CT	C01-C02	3.19	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	605	CHL	CHB-C1B	3.19	1.46	1.39
25	S	616	CLA	C4D-ND	-3.19	1.33	1.37
24	Y	319	CHL	CHB-C1B	3.19	1.46	1.39
24	g	313	CHL	MG-NA	-3.19	1.98	2.06
24	q	304	CHL	CHB-C1B	3.19	1.46	1.39
24	s	414	CHL	CHB-C1B	3.19	1.46	1.39
24	3	308	CHL	MG-NA	-3.18	1.98	2.06
25	N	306	CLA	C4B-NB	3.18	1.41	1.37
25	c	610	CLA	C1D-ND	3.18	1.41	1.37
31	s	415	8CT	C18-C17	3.18	1.53	1.43
24	s	403	CHL	CHD-C4C	3.18	1.46	1.39
24	1	305	CHL	C3D-C2D	3.18	1.47	1.39
24	S	602	CHL	CHD-C4C	3.18	1.46	1.39
25	q	305	CLA	C4D-ND	-3.18	1.33	1.37
24	S	602	CHL	C3D-C2D	3.18	1.47	1.39
24	4	305	CHL	C3D-C2D	3.18	1.47	1.39
24	y	318	CHL	CHB-C1B	3.18	1.46	1.39
24	6	308	CHL	MG-NA	-3.18	1.98	2.06
25	1	307	CLA	C4B-NB	3.18	1.41	1.37
25	4	307	CLA	C4B-NB	3.18	1.41	1.37
31	V	401	8CT	C01-C02	3.18	1.56	1.50
24	4	311	CHL	C3D-C2D	3.18	1.47	1.39
24	q	311	CHL	C3D-C2D	3.18	1.47	1.39
24	p	310	CHL	MG-NA	-3.18	1.98	2.06
24	3	312	CHL	MG-NA	-3.18	1.98	2.06
25	8	305	CLA	C4D-ND	-3.18	1.33	1.37
24	u	309	CHL	MG-NA	-3.18	1.98	2.06
25	r	311	CLA	C4D-ND	-3.18	1.33	1.37
24	6	310	CHL	MG-NA	-3.17	1.98	2.06
24	u	310	CHL	MG-NA	-3.17	1.98	2.06
25	R	609	CLA	C4D-ND	-3.17	1.33	1.37
25	p	314	CLA	C4D-ND	-3.17	1.33	1.37
31	C	615	8CT	C01-C02	3.17	1.56	1.50
24	R	606	CHL	C3D-C2D	3.17	1.47	1.39
24	6	317	CHL	MG-NA	-3.17	1.98	2.06
31	S	614	8CT	C18-C17	3.17	1.53	1.43
25	r	305	CLA	C4D-ND	-3.17	1.33	1.37
24	8	304	CHL	C3D-C2D	3.17	1.47	1.39
25	6	314	CLA	C4B-NB	3.17	1.41	1.37
24	5	306	CHL	CHB-C1B	3.17	1.46	1.39
31	C	615	8CT	C35-C30	3.17	1.65	1.56
24	1	311	CHL	C3D-C2D	3.17	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	313	CLA	C4B-NB	3.17	1.41	1.37
24	G	313	CHL	MG-NA	-3.17	1.98	2.06
24	n	308	CHL	MG-NA	-3.17	1.98	2.06
24	Y	312	CHL	C3D-C2D	3.17	1.47	1.39
24	S	607	CHL	CHB-C1B	3.17	1.46	1.39
25	G	315	CLA	C4B-NB	3.16	1.41	1.37
25	C	616	CLA	C1D-ND	3.16	1.41	1.37
25	b	611	CLA	C1D-ND	3.16	1.41	1.37
24	r	308	CHL	CHB-C1B	3.16	1.46	1.39
24	R	605	CHL	C3D-C2D	3.16	1.47	1.39
24	q	304	CHL	C3D-C2D	3.16	1.47	1.39
24	1	309	CHL	MG-NA	-3.16	1.98	2.06
25	s	404	CLA	C4D-ND	-3.16	1.33	1.37
24	R	607	CHL	CHB-C1B	3.16	1.46	1.39
25	s	410	CLA	C4D-ND	-3.16	1.33	1.37
23	f	201	HEM	FE-NB	3.16	2.04	1.94
24	8	315	CHL	MG-NA	-3.16	1.98	2.06
25	g	317	CLA	C4D-ND	-3.16	1.33	1.37
25	B	603	CLA	C1D-ND	3.16	1.41	1.37
25	g	315	CLA	C4B-NB	3.16	1.41	1.37
24	s	403	CHL	C3D-C2D	3.16	1.47	1.39
24	n	309	CHL	CHB-C1B	3.16	1.46	1.39
25	3	306	CLA	C4B-NB	3.15	1.41	1.37
25	C	610	CLA	C1D-ND	3.15	1.41	1.37
25	b	601	CLA	C4D-ND	-3.15	1.33	1.37
24	9	310	CHL	MG-NA	-3.15	1.98	2.06
24	4	309	CHL	MG-NA	-3.15	1.98	2.06
24	y	313	CHL	C3D-C2D	3.15	1.47	1.39
24	p	305	CHL	CHB-C1B	3.15	1.46	1.39
24	r	302	CHL	MG-NA	-3.15	1.98	2.06
31	S	614	8CT	C01-C02	3.15	1.56	1.50
25	5	314	CLA	C4D-ND	-3.15	1.33	1.37
24	Y	317	CHL	CHB-C1B	3.15	1.46	1.39
24	y	306	CHL	C3D-C2D	3.15	1.47	1.39
24	4	304	CHL	C3A-C2A	-3.14	1.51	1.54
24	8	309	CHL	CHB-C1B	3.14	1.46	1.39
25	s	417	CLA	C4B-NB	3.14	1.41	1.37
24	n	304	CHL	MG-NA	-3.14	1.98	2.06
31	S	615	8CT	C35-C30	3.14	1.65	1.56
24	y	318	CHL	C3D-C2D	3.14	1.47	1.39
25	5	316	CLA	C4D-ND	-3.14	1.33	1.37
25	G	317	CLA	C4B-NB	3.14	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	615	8CT	C10-C03	3.14	1.56	1.45
31	s	416	8CT	C10-C03	3.14	1.56	1.45
24	N	311	CHL	C3D-C2D	3.14	1.47	1.39
25	8	314	CLA	C4B-NB	3.14	1.41	1.37
31	v	401	8CT	C35-C30	3.14	1.65	1.56
24	3	311	CHL	C3D-C2D	3.14	1.47	1.39
31	s	416	8CT	C35-C30	3.14	1.65	1.56
25	p	316	CLA	C4D-ND	-3.14	1.33	1.37
24	n	311	CHL	C3D-C2D	3.14	1.47	1.39
31	c	615	8CT	C01-C02	3.13	1.56	1.50
25	G	314	CLA	C4B-NB	3.13	1.41	1.37
24	6	312	CHL	MG-NA	-3.13	1.98	2.06
24	Y	305	CHL	C3D-C2D	3.13	1.47	1.39
24	2	311	CHL	MG-NA	-3.13	1.98	2.06
24	q	308	CHL	CHB-C1B	3.13	1.46	1.39
24	7	305	CHL	CHB-C1B	3.13	1.46	1.39
24	S	607	CHL	C3D-C2D	3.13	1.47	1.39
24	7	310	CHL	MG-NA	-3.13	1.98	2.06
24	3	310	CHL	MG-NA	-3.13	1.98	2.06
24	3	317	CHL	MG-NA	-3.13	1.98	2.06
24	g	311	CHL	MG-NA	-3.13	1.98	2.06
24	p	306	CHL	C3D-C2D	3.13	1.47	1.39
25	2	307	CLA	C4B-NB	3.13	1.41	1.37
24	N	310	CHL	MG-NA	-3.12	1.98	2.06
24	7	306	CHL	C3D-C2D	3.12	1.47	1.39
25	C	607	CLA	C1D-ND	3.12	1.41	1.37
25	G	317	CLA	C4D-ND	-3.12	1.33	1.37
25	3	307	CLA	C4B-NB	3.12	1.41	1.37
25	c	605	CLA	C1D-ND	3.12	1.41	1.37
24	5	311	CHL	MG-NA	-3.12	1.98	2.06
25	S	609	CLA	C4D-ND	-3.12	1.33	1.37
25	S	616	CLA	C4B-NB	3.12	1.41	1.37
25	B	601	CLA	C4D-ND	-3.12	1.33	1.37
31	V	401	8CT	C35-C30	3.12	1.65	1.56
24	2	312	CHL	C3D-C2D	3.12	1.47	1.39
24	N	304	CHL	MG-NA	-3.12	1.98	2.06
25	g	317	CLA	C4B-NB	3.12	1.41	1.37
25	c	616	CLA	C1D-ND	3.12	1.41	1.37
31	B	617	8CT	C01-C02	3.12	1.56	1.50
25	g	314	CLA	C4B-NB	3.11	1.41	1.37
31	T	101	8CT	C01-C02	3.11	1.56	1.50
31	b	617	8CT	C18-C17	3.11	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	311	CLA	C4D-ND	-3.11	1.33	1.37
25	g	316	CLA	C4B-NB	3.11	1.41	1.37
31	d	410	8CT	C35-C30	3.11	1.65	1.56
25	r	310	CLA	C4D-ND	-3.11	1.33	1.37
31	c	615	8CT	C18-C17	3.11	1.53	1.43
25	7	307	CLA	C4D-ND	-3.11	1.33	1.37
24	g	310	CHL	MG-NA	-3.11	1.98	2.06
24	q	316	CHL	MG-NA	-3.11	1.98	2.06
24	y	312	CHL	CHB-C1B	3.11	1.46	1.39
31	b	617	8CT	C01-C02	3.11	1.56	1.50
24	y	311	CHL	C3D-C2D	3.11	1.47	1.39
24	R	602	CHL	C3D-C2D	3.11	1.47	1.39
24	r	303	CHL	C3D-C2D	3.11	1.47	1.39
24	S	601	CHL	CHB-C1B	3.11	1.46	1.39
25	p	308	CLA	C4B-NB	3.11	1.41	1.37
24	6	311	CHL	C3D-C2D	3.11	1.47	1.39
24	s	408	CHL	C3D-C2D	3.11	1.47	1.39
25	q	312	CLA	C4D-ND	-3.10	1.33	1.37
24	8	310	CHL	CHB-C1B	3.10	1.46	1.39
25	q	315	CLA	C4B-NB	3.10	1.41	1.37
31	A	608	8CT	C35-C30	3.10	1.65	1.56
31	D	410	8CT	C35-C30	3.10	1.65	1.56
24	q	309	CHL	C3D-C2D	3.10	1.47	1.39
24	s	402	CHL	CHB-C1B	3.10	1.46	1.39
24	u	311	CHL	MG-NA	-3.10	1.98	2.06
25	5	307	CLA	C4B-NB	3.10	1.41	1.37
24	q	311	CHL	CHB-C1B	3.10	1.46	1.39
25	3	306	CLA	C4D-ND	-3.10	1.33	1.37
25	p	307	CLA	C4D-ND	-3.10	1.33	1.37
25	R	610	CLA	C4D-ND	-3.10	1.33	1.37
25	8	306	CLA	C4B-NB	3.10	1.41	1.37
25	r	312	CLA	C4D-ND	-3.10	1.33	1.37
24	n	310	CHL	MG-NA	-3.09	1.98	2.06
31	a	608	8CT	C35-C30	3.09	1.65	1.56
24	Y	317	CHL	C3D-C2D	3.09	1.47	1.39
25	R	604	CLA	C4D-ND	-3.09	1.33	1.37
25	n	306	CLA	C4D-ND	-3.09	1.33	1.37
25	1	306	CLA	C4B-NB	3.09	1.41	1.37
25	2	314	CLA	C4D-ND	-3.09	1.33	1.37
31	S	615	8CT	C18-C17	3.09	1.53	1.43
24	1	304	CHL	C3A-C2A	-3.09	1.51	1.54
25	1	307	CLA	C4D-ND	-3.09	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	312	CLA	C4B-NB	3.09	1.41	1.37
24	9	309	CHL	MG-NA	-3.09	1.98	2.06
25	2	316	CLA	C4D-ND	-3.09	1.33	1.37
24	Y	310	CHL	C3D-C2D	3.09	1.47	1.39
31	C	613	8CT	C07-C02	-3.08	1.44	1.51
24	9	304	CHL	MG-NA	-3.08	1.98	2.06
31	s	415	8CT	C10-C03	3.08	1.56	1.45
25	p	308	CLA	C4D-ND	-3.08	1.33	1.37
24	S	613	CHL	C3D-C2D	3.08	1.47	1.39
24	s	414	CHL	C3D-C2D	3.08	1.47	1.39
24	n	317	CHL	C3A-C2A	-3.08	1.51	1.54
31	C	615	8CT	C18-C17	3.08	1.53	1.43
31	t	101	8CT	C01-C02	3.08	1.56	1.50
24	Y	311	CHL	CHB-C1B	3.08	1.46	1.39
25	2	315	CLA	C4D-ND	-3.08	1.33	1.37
25	5	315	CLA	C4D-ND	-3.08	1.33	1.37
24	G	310	CHL	MG-NA	-3.08	1.99	2.06
24	y	305	CHL	CHB-C1B	3.08	1.46	1.39
25	R	611	CLA	C4D-ND	-3.08	1.33	1.37
31	c	613	8CT	C07-C02	-3.08	1.44	1.51
25	7	308	CLA	C4B-NB	3.08	1.41	1.37
24	8	307	CHL	MG-NA	-3.08	1.99	2.06
24	q	307	CHL	MG-NA	-3.07	1.99	2.06
25	R	604	CLA	C4B-NB	3.07	1.41	1.37
25	q	313	CLA	C4B-NB	3.07	1.41	1.37
25	r	305	CLA	C4B-NB	3.07	1.41	1.37
24	Y	311	CHL	C3D-C2D	3.07	1.47	1.39
25	C	605	CLA	C1D-ND	3.07	1.41	1.37
31	S	614	8CT	C10-C03	3.07	1.56	1.45
24	p	318	CHL	MG-NA	-3.07	1.99	2.06
24	4	317	CHL	C3A-C2A	-3.07	1.51	1.54
31	S	614	8CT	C35-C30	3.07	1.64	1.56
25	8	312	CLA	C4D-ND	-3.07	1.33	1.37
35	d	403	PHO	C4D-CHA	3.06	1.44	1.39
31	B	617	8CT	C18-C17	3.06	1.52	1.43
24	Y	304	CHL	CHB-C1B	3.06	1.46	1.39
25	g	307	CLA	C4D-ND	-3.06	1.33	1.37
24	5	312	CHL	C3D-C2D	3.06	1.47	1.39
25	4	307	CLA	C4D-ND	-3.06	1.33	1.37
24	y	312	CHL	C3D-C2D	3.06	1.47	1.39
25	6	306	CLA	C4B-NB	3.06	1.41	1.37
25	7	307	CLA	C4B-NB	3.06	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	311	CHL	MG-NA	-3.06	1.99	2.06
25	5	307	CLA	C4D-ND	-3.06	1.33	1.37
31	s	416	8CT	C18-C17	3.06	1.52	1.43
25	8	313	CLA	C4D-ND	-3.06	1.33	1.37
25	G	315	CLA	C4D-ND	-3.06	1.33	1.37
24	Y	319	CHL	C3D-C2D	3.05	1.47	1.39
24	y	311	CHL	CHB-C1B	3.05	1.46	1.39
32	a	609	SQD	O48-C23	3.05	1.42	1.33
25	5	315	CLA	C4B-NB	3.05	1.41	1.37
24	8	308	CHL	C3D-C2D	3.05	1.47	1.39
24	6	304	CHL	MG-NA	-3.05	1.99	2.06
25	5	316	CLA	C4B-NB	3.05	1.41	1.37
25	2	308	CLA	C4D-ND	-3.05	1.33	1.37
25	6	313	CLA	C4D-ND	-3.05	1.33	1.37
24	2	313	CHL	MG-NA	-3.05	1.99	2.06
24	1	317	CHL	C3A-C2A	-3.05	1.51	1.54
32	b	618	SQD	O48-C23	3.05	1.42	1.33
24	7	318	CHL	MG-NA	-3.05	1.99	2.06
25	3	313	CLA	C4D-ND	-3.05	1.33	1.37
25	r	304	CLA	C4D-ND	-3.05	1.33	1.37
31	T	101	8CT	C18-C17	3.05	1.52	1.43
25	N	306	CLA	C4D-ND	-3.05	1.33	1.37
31	s	415	8CT	C35-C30	3.05	1.64	1.56
24	s	402	CHL	C3D-C2D	3.05	1.47	1.39
25	R	603	CLA	C4D-ND	-3.05	1.33	1.37
25	B	606	CLA	C1D-ND	3.05	1.41	1.37
32	A	609	SQD	O48-C23	3.05	1.42	1.33
25	G	316	CLA	C4D-ND	-3.04	1.33	1.37
25	g	315	CLA	C4D-ND	-3.04	1.33	1.37
25	2	315	CLA	C4B-NB	3.04	1.41	1.37
25	2	316	CLA	C4B-NB	3.04	1.41	1.37
25	3	316	CLA	C4D-ND	-3.04	1.33	1.37
24	N	317	CHL	C3A-C2A	-3.04	1.51	1.54
24	Y	310	CHL	CHB-C1B	3.04	1.46	1.39
32	B	618	SQD	O48-C23	3.04	1.42	1.33
25	a	604	CLA	C4B-NB	3.04	1.41	1.37
25	S	604	CLA	C4B-NB	3.04	1.41	1.37
25	q	306	CLA	C4B-NB	3.04	1.41	1.37
24	q	308	CHL	C3D-C2D	3.04	1.47	1.39
24	n	309	CHL	C3D-C2D	3.04	1.47	1.39
25	q	315	CLA	C4D-ND	-3.04	1.33	1.37
31	t	101	8CT	C18-C17	3.04	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	601	CHL	C3D-C2D	3.04	1.47	1.39
24	y	310	CHL	CHB-C1B	3.04	1.46	1.39
24	N	309	CHL	C3D-C2D	3.03	1.47	1.39
25	q	314	CLA	C4D-ND	-3.03	1.33	1.37
31	V	401	8CT	C18-C17	3.03	1.52	1.43
24	r	309	CHL	MG-NA	-3.03	1.99	2.06
25	s	405	CLA	C4B-NB	3.03	1.41	1.37
24	4	312	CHL	MG-NA	-3.03	1.99	2.06
25	q	313	CLA	C4D-ND	-3.03	1.33	1.37
25	s	411	CLA	O1A-CGA	3.03	1.37	1.19
25	6	306	CLA	C4D-ND	-3.03	1.33	1.37
31	v	401	8CT	C18-C17	3.03	1.52	1.43
25	2	317	CLA	C4D-ND	-3.03	1.33	1.37
24	N	308	CHL	MG-NA	-3.03	1.99	2.06
24	7	311	CHL	MG-NA	-3.03	1.99	2.06
35	D	403	PHO	C4D-CHA	3.03	1.44	1.39
25	b	606	CLA	C1D-ND	3.03	1.41	1.37
24	7	312	CHL	C3D-C2D	3.03	1.47	1.39
25	1	306	CLA	C4D-ND	-3.03	1.33	1.37
25	7	315	CLA	C4B-NB	3.03	1.41	1.37
25	b	609	CLA	C4B-NB	3.02	1.41	1.37
25	3	315	CLA	C4D-ND	-3.02	1.33	1.37
31	C	613	8CT	C18-C17	3.02	1.52	1.43
24	1	312	CHL	MG-NA	-3.02	1.99	2.06
24	q	309	CHL	MG-NA	-3.02	1.99	2.06
24	7	305	CHL	C3D-C2D	3.02	1.47	1.39
25	R	613	CLA	C3B-C4B	3.02	1.49	1.42
25	q	314	CLA	C4B-NB	3.02	1.41	1.37
25	n	307	CLA	C4D-ND	-3.01	1.33	1.37
25	4	306	CLA	C4D-ND	-3.01	1.33	1.37
25	7	308	CLA	C4D-ND	-3.01	1.33	1.37
31	x	601	8CT	C35-C30	3.01	1.64	1.56
24	8	309	CHL	C3D-C2D	3.01	1.47	1.39
25	p	315	CLA	C4B-NB	3.01	1.41	1.37
24	2	305	CHL	MG-NA	-3.01	1.99	2.06
24	p	311	CHL	MG-NA	-3.01	1.99	2.06
23	f	201	HEM	CAB-C3B	3.01	1.55	1.47
24	q	310	CHL	C3D-C2D	3.01	1.47	1.39
25	B	605	CLA	C4B-NB	3.01	1.41	1.37
25	9	306	CLA	C4D-ND	-3.01	1.33	1.37
25	4	314	CLA	C4D-ND	-3.01	1.33	1.37
25	p	317	CLA	C4D-ND	-3.01	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	603	CLA	C4B-NB	3.01	1.41	1.37
25	p	307	CLA	C4B-NB	3.01	1.41	1.37
24	y	309	CHL	MG-NA	-3.01	1.99	2.06
25	r	304	CLA	C4B-NB	3.01	1.41	1.37
31	C	613	8CT	C01-C02	3.01	1.55	1.50
25	5	308	CLA	C4D-ND	-3.01	1.33	1.37
25	1	315	CLA	C4D-ND	-3.01	1.33	1.37
25	G	307	CLA	C4D-ND	-3.01	1.33	1.37
25	b	605	CLA	C4B-NB	3.00	1.41	1.37
25	2	307	CLA	C4D-ND	-3.00	1.33	1.37
25	g	314	CLA	C4D-ND	-3.00	1.33	1.37
25	r	312	CLA	C4B-NB	3.00	1.41	1.37
25	a	604	CLA	C3B-C4B	3.00	1.49	1.42
25	3	307	CLA	C4D-ND	-3.00	1.33	1.37
32	D	409	SQD	O48-C23	3.00	1.42	1.33
25	g	316	CLA	C4D-ND	-3.00	1.33	1.37
24	3	309	CHL	MG-NA	-3.00	1.99	2.06
32	d	409	SQD	O48-C23	3.00	1.42	1.33
24	Y	308	CHL	MG-NA	-3.00	1.99	2.06
24	Y	309	CHL	CHB-C1B	2.99	1.46	1.39
25	N	307	CLA	C4D-ND	-2.99	1.33	1.37
24	R	608	CHL	MG-NA	-2.99	1.99	2.06
24	p	312	CHL	C3D-C2D	2.99	1.47	1.39
25	n	315	CLA	C4D-ND	-2.99	1.33	1.37
31	c	613	8CT	C18-C17	2.99	1.52	1.43
25	2	308	CLA	C4B-NB	2.99	1.41	1.37
25	8	313	CLA	C4B-NB	2.99	1.41	1.37
25	C	604	CLA	C4B-NB	2.99	1.41	1.37
25	N	315	CLA	C4D-ND	-2.99	1.33	1.37
25	G	308	CLA	C4D-ND	-2.99	1.33	1.37
25	d	404	CLA	C1D-ND	2.99	1.41	1.37
25	B	609	CLA	C4B-NB	2.99	1.41	1.37
25	s	404	CLA	C4B-NB	2.99	1.41	1.37
24	p	305	CHL	C3D-C2D	2.99	1.47	1.39
39	d	406	PL9	C53-C6	-2.99	1.44	1.50
31	X	601	8CT	C35-C30	2.99	1.64	1.56
24	6	309	CHL	MG-NA	-2.98	1.99	2.06
25	R	612	CLA	C4D-ND	-2.98	1.33	1.37
25	6	316	CLA	C4D-ND	-2.98	1.33	1.37
31	B	617	8CT	C35-C30	2.98	1.64	1.56
31	T	101	8CT	C07-C02	-2.98	1.45	1.51
25	4	315	CLA	C4D-ND	-2.98	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	604	CLA	C3B-C4B	2.98	1.49	1.42
25	1	314	CLA	C4D-ND	-2.98	1.33	1.37
31	c	614	8CT	C01-C02	2.98	1.55	1.50
24	5	313	CHL	MG-NA	-2.98	1.99	2.06
31	C	615	8CT	C10-C03	2.98	1.55	1.45
24	3	305	CHL	MG-NA	-2.98	1.99	2.06
24	Y	319	CHL	MG-NA	-2.98	1.99	2.06
25	u	307	CLA	C4D-ND	-2.98	1.33	1.37
25	1	313	CLA	C4D-ND	-2.98	1.33	1.37
31	A	608	8CT	C18-C17	2.98	1.52	1.43
31	d	410	8CT	C18-C17	2.98	1.52	1.43
25	R	611	CLA	C4B-NB	2.98	1.41	1.37
25	6	315	CLA	C4D-ND	-2.98	1.33	1.37
25	5	314	CLA	C4B-NB	2.98	1.41	1.37
24	y	305	CHL	C3D-C2D	2.98	1.47	1.39
24	Y	305	CHL	CHB-C1B	2.97	1.46	1.39
25	5	308	CLA	C4B-NB	2.97	1.41	1.37
24	5	305	CHL	MG-NA	-2.97	1.99	2.06
24	r	306	CHL	MG-NA	-2.97	1.99	2.06
25	r	313	CLA	C4D-ND	-2.97	1.33	1.37
25	N	313	CLA	C4D-ND	-2.97	1.33	1.37
25	7	317	CLA	C4D-ND	-2.97	1.33	1.37
25	R	603	CLA	C4B-NB	2.97	1.41	1.37
31	c	613	8CT	C01-C02	2.97	1.55	1.50
24	p	306	CHL	CHB-C1B	2.97	1.46	1.39
25	3	316	CLA	C3B-C4B	2.96	1.49	1.42
31	S	615	8CT	C01-C02	2.96	1.55	1.50
25	D	404	CLA	C1D-ND	2.96	1.41	1.37
25	4	313	CLA	C4D-ND	-2.96	1.33	1.37
25	u	308	CLA	C4D-ND	-2.96	1.33	1.37
24	y	306	CHL	CHB-C1B	2.96	1.46	1.39
25	q	312	CLA	C4B-NB	2.96	1.41	1.37
31	a	608	8CT	C18-C17	2.96	1.52	1.43
25	1	313	CLA	C3B-C4B	2.96	1.49	1.42
25	r	314	CLA	C3B-C4B	2.96	1.49	1.42
25	6	307	CLA	C4D-ND	-2.96	1.33	1.37
25	p	315	CLA	C4D-ND	-2.96	1.33	1.37
25	2	314	CLA	C4B-NB	2.96	1.41	1.37
31	c	615	8CT	C10-C03	2.96	1.55	1.45
31	D	410	8CT	C18-C17	2.96	1.52	1.43
25	A	604	CLA	C4B-NB	2.96	1.41	1.37
25	7	315	CLA	C4D-ND	-2.96	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	612	CLA	C4B-NB	2.96	1.41	1.37
25	B	615	CLA	C4B-NB	2.96	1.41	1.37
25	n	313	CLA	C4D-ND	-2.96	1.33	1.37
31	c	614	8CT	C18-C17	2.96	1.52	1.43
31	X	601	8CT	C18-C17	2.96	1.52	1.43
25	G	314	CLA	C4D-ND	-2.95	1.33	1.37
25	4	316	CLA	C4D-ND	-2.95	1.33	1.37
25	g	308	CLA	C4D-ND	-2.95	1.33	1.37
25	3	314	CLA	C4D-ND	-2.95	1.33	1.37
25	5	317	CLA	C4D-ND	-2.95	1.33	1.37
24	y	310	CHL	C3D-C2D	2.95	1.47	1.39
23	E	201	HEM	CAB-C3B	2.95	1.55	1.47
25	3	313	CLA	C3B-C4B	2.95	1.49	1.42
25	B	607	CLA	C4B-NB	2.95	1.41	1.37
25	b	607	CLA	C4B-NB	2.95	1.41	1.37
25	8	314	CLA	C4D-ND	-2.95	1.33	1.37
23	E	201	HEM	CAC-C3C	2.95	1.55	1.47
25	N	313	CLA	C3B-C4B	2.95	1.49	1.42
25	p	316	CLA	C4B-NB	2.95	1.41	1.37
31	t	101	8CT	C07-C02	-2.95	1.45	1.51
25	s	413	CLA	C4B-NB	2.95	1.41	1.37
24	s	402	CHL	MG-NA	-2.95	1.99	2.06
24	7	306	CHL	CHB-C1B	2.95	1.46	1.39
25	5	317	CLA	C4B-NB	2.95	1.41	1.37
25	4	313	CLA	C3B-C4B	2.94	1.49	1.42
25	6	314	CLA	C4D-ND	-2.94	1.33	1.37
25	q	305	CLA	C4B-NB	2.94	1.41	1.37
24	Y	309	CHL	C3D-C2D	2.94	1.47	1.39
25	b	615	CLA	C4B-NB	2.94	1.41	1.37
25	9	313	CLA	C3B-C4B	2.94	1.49	1.42
24	g	305	CHL	MG-NA	-2.94	1.99	2.06
25	N	314	CLA	C4D-ND	-2.94	1.33	1.37
25	9	314	CLA	C3B-C4B	2.94	1.49	1.42
25	9	315	CLA	C4D-ND	-2.94	1.33	1.37
24	s	414	CHL	MG-NA	-2.94	1.99	2.06
24	3	304	CHL	MG-NA	-2.94	1.99	2.06
25	N	316	CLA	C4D-ND	-2.94	1.33	1.37
31	s	416	8CT	C01-C02	2.94	1.55	1.50
24	s	403	CHL	MG-NA	-2.94	1.99	2.06
25	n	313	CLA	C3B-C4B	2.94	1.49	1.42
25	b	608	CLA	C4B-NB	2.93	1.41	1.37
25	u	314	CLA	C3B-C4B	2.93	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	304	CHL	C3D-C2D	2.93	1.47	1.39
25	p	314	CLA	C4B-NB	2.93	1.41	1.37
23	f	201	HEM	CAC-C3C	2.93	1.55	1.47
31	C	614	8CT	C01-C02	2.93	1.55	1.50
25	R	610	CLA	C4B-NB	2.93	1.41	1.37
25	u	315	CLA	C3B-C4B	2.93	1.49	1.42
31	x	601	8CT	C18-C17	2.93	1.52	1.43
24	7	313	CHL	MG-NA	-2.93	1.99	2.06
31	b	617	8CT	C35-C30	2.93	1.64	1.56
31	X	601	8CT	C30-C29	2.93	1.54	1.50
25	4	314	CLA	C3B-C4B	2.93	1.49	1.42
31	x	601	8CT	C30-C29	2.93	1.54	1.50
24	p	313	CHL	MG-NA	-2.93	1.99	2.06
31	B	617	8CT	C10-C03	2.93	1.55	1.45
31	v	401	8CT	C30-C29	2.93	1.54	1.50
31	C	614	8CT	C18-C17	2.92	1.52	1.43
25	n	314	CLA	C4D-ND	-2.92	1.33	1.37
25	8	305	CLA	C4B-NB	2.92	1.41	1.37
25	8	311	CLA	C4B-NB	2.92	1.41	1.37
25	u	316	CLA	C4D-ND	-2.92	1.33	1.37
25	9	307	CLA	C4D-ND	-2.92	1.33	1.37
25	u	317	CLA	C4D-ND	-2.92	1.33	1.37
25	6	313	CLA	C3B-C4B	2.92	1.49	1.42
24	y	313	CHL	MG-NA	-2.92	1.99	2.06
25	9	316	CLA	C3B-C4B	2.92	1.49	1.42
31	b	617	8CT	C10-C03	2.92	1.55	1.45
25	7	316	CLA	C4B-NB	2.92	1.41	1.37
24	S	613	CHL	MG-NA	-2.92	1.99	2.06
39	D	406	PL9	C53-C6	-2.92	1.44	1.50
24	S	606	CHL	MG-NA	-2.92	1.99	2.06
31	d	410	8CT	C10-C03	2.92	1.55	1.45
25	r	310	CLA	C4B-NB	2.92	1.41	1.37
31	V	401	8CT	C30-C29	2.92	1.54	1.50
25	n	316	CLA	C4D-ND	-2.92	1.33	1.37
25	1	316	CLA	C4D-ND	-2.92	1.33	1.37
25	2	317	CLA	C4B-NB	2.92	1.41	1.37
24	6	305	CHL	MG-NA	-2.91	1.99	2.06
24	u	312	CHL	MG-NA	-2.91	1.99	2.06
25	s	412	CLA	C4B-NB	2.91	1.41	1.37
24	G	305	CHL	MG-NA	-2.91	1.99	2.06
25	6	316	CLA	C3B-C4B	2.91	1.49	1.42
24	R	602	CHL	MG-NA	-2.91	1.99	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	310	CHL	MG-NA	-2.91	1.99	2.06
24	r	307	CHL	MG-NA	-2.90	1.99	2.06
25	u	317	CLA	C3B-C4B	2.90	1.49	1.42
24	r	308	CHL	C3D-C2D	2.90	1.47	1.39
30	D	408	LHG	C26-C25	-2.90	1.35	1.51
25	Y	314	CLA	C4B-NB	2.90	1.41	1.37
25	r	314	CLA	C4D-ND	-2.90	1.33	1.37
25	r	311	CLA	C4B-NB	2.90	1.41	1.37
30	D	407	LHG	C26-C25	-2.90	1.35	1.51
24	R	607	CHL	C3D-C2D	2.90	1.47	1.39
25	b	601	CLA	C4B-NB	2.90	1.41	1.37
35	a	606	PHO	C4D-CHA	2.90	1.44	1.39
30	d	407	LHG	C26-C25	-2.90	1.35	1.51
24	n	312	CHL	MG-NA	-2.90	1.99	2.06
25	b	616	CLA	C4B-NB	2.90	1.41	1.37
25	4	315	CLA	C3B-C4B	2.90	1.49	1.42
24	r	303	CHL	MG-NA	-2.90	1.99	2.06
24	4	310	CHL	MG-NA	-2.89	1.99	2.06
30	Y	318	LHG	C26-C25	-2.89	1.35	1.51
24	N	312	CHL	MG-NA	-2.89	1.99	2.06
25	S	610	CLA	C4B-NB	2.89	1.41	1.37
35	A	606	PHO	C4D-CHA	2.89	1.44	1.39
31	X	601	8CT	C07-C02	-2.89	1.45	1.51
24	s	407	CHL	MG-NA	-2.89	1.99	2.06
25	R	613	CLA	C4D-ND	-2.89	1.33	1.37
25	u	315	CLA	C4D-ND	-2.89	1.33	1.37
24	u	306	CHL	MG-NA	-2.89	1.99	2.06
31	D	410	8CT	C10-C03	2.89	1.55	1.45
24	G	312	CHL	MG-NA	-2.89	1.99	2.06
24	S	601	CHL	MG-NA	-2.89	1.99	2.06
24	Y	317	CHL	MG-NA	-2.89	1.99	2.06
31	C	613	8CT	C10-C03	2.88	1.55	1.45
31	c	613	8CT	C10-C03	2.88	1.55	1.45
25	1	315	CLA	C3B-C4B	2.88	1.49	1.42
30	A	601	LHG	C26-C25	-2.88	1.35	1.51
24	1	305	CHL	MG-NA	-2.88	1.99	2.06
32	a	609	SQD	O47-C7	2.88	1.42	1.34
25	a	610	CLA	C4D-ND	-2.88	1.33	1.37
32	A	609	SQD	O47-C7	2.88	1.42	1.34
30	y	319	LHG	C26-C25	-2.88	1.35	1.51
30	a	601	LHG	C26-C25	-2.88	1.35	1.51
25	u	314	CLA	C4D-ND	-2.88	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	610	CLA	C3B-C4B	2.88	1.49	1.42
25	Y	307	CLA	C4B-NB	2.88	1.41	1.37
25	B	608	CLA	C4B-NB	2.88	1.41	1.37
24	4	305	CHL	MG-NA	-2.88	1.99	2.06
25	6	315	CLA	C3B-C4B	2.88	1.49	1.42
24	y	318	CHL	MG-NA	-2.88	1.99	2.06
31	d	410	8CT	C30-C29	2.88	1.54	1.50
25	B	610	CLA	C4B-NB	2.88	1.41	1.37
25	b	610	CLA	C4B-NB	2.88	1.41	1.37
24	Y	312	CHL	MG-NA	-2.88	1.99	2.06
31	x	601	8CT	C07-C02	-2.88	1.45	1.51
30	a	612	LHG	C26-C25	-2.87	1.35	1.51
25	B	611	CLA	C4B-NB	2.87	1.41	1.37
24	9	311	CHL	MG-NA	-2.87	1.99	2.06
25	c	604	CLA	C4B-NB	2.87	1.41	1.37
32	b	618	SQD	O47-C7	2.87	1.42	1.34
25	3	314	CLA	C3B-C4B	2.87	1.49	1.42
31	D	410	8CT	C30-C29	2.87	1.54	1.50
24	G	318	CHL	MG-NA	-2.87	1.99	2.06
25	9	316	CLA	C4D-ND	-2.87	1.33	1.37
30	A	612	LHG	C26-C25	-2.87	1.35	1.51
32	d	409	SQD	O47-C7	2.86	1.42	1.34
25	1	314	CLA	C3B-C4B	2.86	1.49	1.42
24	s	406	CHL	MG-NA	-2.86	1.99	2.06
24	s	408	CHL	MG-NA	-2.86	1.99	2.06
25	S	611	CLA	C4B-NB	2.86	1.41	1.37
25	3	315	CLA	C3B-C4B	2.86	1.49	1.42
25	4	316	CLA	C3B-C4B	2.86	1.49	1.42
24	9	305	CHL	MG-NA	-2.86	1.99	2.06
25	R	609	CLA	C4B-NB	2.86	1.41	1.37
25	B	601	CLA	C4B-NB	2.86	1.41	1.37
24	8	310	CHL	MG-NA	-2.86	1.99	2.06
24	S	602	CHL	MG-NA	-2.86	1.99	2.06
24	g	318	CHL	MG-NA	-2.86	1.99	2.06
24	s	409	CHL	MG-NA	-2.86	1.99	2.06
31	v	401	8CT	C07-C02	-2.86	1.45	1.51
32	B	618	SQD	O47-C7	2.85	1.42	1.34
25	B	602	CLA	C4B-NB	2.85	1.41	1.37
25	g	314	CLA	C3B-C4B	2.85	1.49	1.42
25	9	313	CLA	C4D-ND	-2.85	1.33	1.37
25	y	308	CLA	C4B-NB	2.85	1.41	1.37
25	7	314	CLA	C4B-NB	2.85	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	C4B-NB	2.85	1.41	1.37
30	7	319	LHG	C26-C25	-2.85	1.35	1.51
31	T	101	8CT	C10-C03	2.85	1.55	1.45
24	5	306	CHL	MG-NA	-2.85	1.99	2.06
30	C	617	LHG	C26-C25	-2.84	1.35	1.51
25	R	612	CLA	C3B-C4B	2.84	1.49	1.42
25	y	315	CLA	C4B-NB	2.84	1.41	1.37
25	A	610	CLA	C4D-ND	-2.84	1.33	1.37
31	t	101	8CT	C10-C03	2.84	1.55	1.45
25	9	315	CLA	C3B-C4B	2.84	1.49	1.42
24	q	304	CHL	MG-NA	-2.84	1.99	2.06
25	6	314	CLA	C3B-C4B	2.84	1.49	1.42
24	2	306	CHL	MG-NA	-2.84	1.99	2.06
30	p	319	LHG	C26-C25	-2.84	1.35	1.51
25	D	405	CLA	C4B-NB	2.83	1.41	1.37
24	q	311	CHL	MG-NA	-2.83	1.99	2.06
32	D	409	SQD	O47-C7	2.83	1.42	1.34
30	c	617	LHG	C26-C25	-2.83	1.35	1.51
25	g	317	CLA	C3B-C4B	2.83	1.49	1.42
25	B	616	CLA	C4B-NB	2.83	1.41	1.37
30	5	319	LHG	C26-C25	-2.83	1.35	1.51
31	A	608	8CT	C10-C03	2.83	1.55	1.45
30	g	319	LHG	C26-C25	-2.83	1.35	1.51
25	G	308	CLA	C3B-C4B	2.83	1.49	1.42
25	Y	316	CLA	C4B-NB	2.83	1.41	1.37
25	1	316	CLA	C3B-C4B	2.83	1.49	1.42
25	u	316	CLA	C3B-C4B	2.83	1.49	1.42
25	n	314	CLA	C3B-C4B	2.83	1.49	1.42
30	2	319	LHG	C26-C25	-2.83	1.35	1.51
31	V	401	8CT	C10-C03	2.83	1.55	1.45
25	2	315	CLA	C3B-C4B	2.83	1.49	1.42
30	n	318	LHG	C26-C25	-2.83	1.35	1.51
25	N	316	CLA	C3B-C4B	2.83	1.49	1.42
25	1	306	CLA	C3B-C4B	2.83	1.49	1.42
25	n	316	CLA	C3B-C4B	2.83	1.49	1.42
31	X	601	8CT	C10-C03	2.82	1.55	1.45
25	G	314	CLA	C3B-C4B	2.82	1.49	1.42
24	S	607	CHL	MG-NA	-2.82	1.99	2.06
25	y	317	CLA	C4B-NB	2.82	1.41	1.37
25	a	610	CLA	C3B-C4B	2.82	1.49	1.42
24	3	311	CHL	C3B-C4B	2.82	1.49	1.42
31	a	608	8CT	C10-C03	2.82	1.55	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	311	CHL	MG-NA	-2.82	1.99	2.06
25	d	405	CLA	C4B-NB	2.82	1.41	1.37
30	G	319	LHG	C26-C25	-2.82	1.35	1.51
24	8	304	CHL	MG-NA	-2.82	1.99	2.06
25	B	604	CLA	C4B-NB	2.82	1.41	1.37
25	B	614	CLA	C4B-NB	2.82	1.41	1.37
25	G	317	CLA	C3B-C4B	2.82	1.49	1.42
25	s	410	CLA	C4B-NB	2.82	1.41	1.37
24	9	309	CHL	C3B-C4B	2.82	1.49	1.42
25	g	315	CLA	C3B-C4B	2.81	1.49	1.42
31	A	608	8CT	C07-C02	-2.81	1.45	1.51
25	R	609	CLA	C3B-C4B	2.81	1.49	1.42
25	G	307	CLA	C3B-C4B	2.81	1.49	1.42
30	N	318	LHG	C26-C25	-2.81	1.35	1.51
24	S	608	CHL	MG-NA	-2.81	1.99	2.06
25	n	307	CLA	C3B-C4B	2.81	1.49	1.42
25	S	609	CLA	C4B-NB	2.81	1.41	1.37
23	E	201	HEM	FE-NB	2.81	2.03	1.94
25	G	307	CLA	C1B-C2B	2.81	1.49	1.43
30	9	318	LHG	C26-C25	-2.81	1.35	1.51
25	5	315	CLA	C3B-C4B	2.81	1.49	1.42
31	a	608	8CT	C07-C02	-2.81	1.45	1.51
31	v	401	8CT	C10-C03	2.80	1.55	1.45
25	3	307	CLA	C3B-C4B	2.80	1.49	1.42
24	R	606	CHL	MG-NA	-2.80	1.99	2.06
24	3	311	CHL	MG-NA	-2.80	1.99	2.06
25	b	613	CLA	C4B-NB	2.80	1.41	1.37
25	5	308	CLA	C3B-C4B	2.80	1.49	1.42
25	C	609	CLA	C3B-C4B	2.80	1.49	1.42
24	q	308	CHL	MG-NA	-2.80	1.99	2.06
30	1	318	LHG	C26-C25	-2.80	1.35	1.51
25	b	602	CLA	C4B-NB	2.80	1.41	1.37
25	y	307	CLA	C4B-NB	2.80	1.41	1.37
24	4	309	CHL	C3B-C4B	2.80	1.49	1.42
25	G	315	CLA	C3B-C4B	2.80	1.49	1.42
25	g	308	CLA	C3B-C4B	2.80	1.49	1.42
35	a	606	PHO	CMC-C2C	-2.80	1.46	1.50
25	9	314	CLA	C4D-ND	-2.80	1.33	1.37
25	6	307	CLA	C3B-C4B	2.80	1.49	1.42
25	s	410	CLA	C3B-C4B	2.80	1.49	1.42
24	S	605	CHL	MG-NA	-2.80	1.99	2.06
24	9	308	CHL	C4D-CHA	2.80	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	614	8CT	C10-C03	2.79	1.55	1.45
30	4	318	LHG	C26-C25	-2.79	1.35	1.51
31	c	615	8CT	C30-C29	2.79	1.54	1.50
31	x	601	8CT	C10-C03	2.79	1.55	1.45
24	u	310	CHL	C3B-C4B	2.79	1.49	1.42
25	s	417	CLA	C3B-C4B	2.79	1.49	1.42
25	p	308	CLA	C3B-C4B	2.79	1.49	1.42
25	c	609	CLA	C3B-C4B	2.79	1.49	1.42
24	G	306	CHL	MG-NA	-2.79	1.99	2.06
25	g	307	CLA	C1B-C2B	2.79	1.49	1.43
25	R	610	CLA	C3B-C4B	2.79	1.49	1.42
24	Y	305	CHL	MG-NA	-2.79	1.99	2.06
24	g	312	CHL	MG-NA	-2.79	1.99	2.06
24	6	311	CHL	C3B-C4B	2.79	1.49	1.42
25	N	307	CLA	C3B-C4B	2.79	1.49	1.42
25	u	308	CLA	C3B-C4B	2.79	1.49	1.42
25	r	310	CLA	C3B-C4B	2.79	1.49	1.42
24	N	317	CHL	C4D-CHA	2.79	1.48	1.38
25	u	307	CLA	C3B-C4B	2.79	1.49	1.42
31	C	614	8CT	C10-C03	2.78	1.55	1.45
25	7	317	CLA	C3B-C4B	2.78	1.49	1.42
31	V	401	8CT	C07-C02	-2.78	1.45	1.51
25	N	314	CLA	C3B-C4B	2.78	1.49	1.42
25	b	614	CLA	C4B-NB	2.78	1.41	1.37
25	s	411	CLA	C4B-NB	2.78	1.41	1.37
25	S	609	CLA	C3B-C4B	2.78	1.49	1.42
25	p	317	CLA	C3B-C4B	2.78	1.49	1.42
24	7	309	CHL	C4D-CHA	2.78	1.48	1.38
25	y	314	CLA	C4B-NB	2.78	1.41	1.37
24	2	310	CHL	MG-NA	-2.78	1.99	2.06
31	C	615	8CT	C30-C29	2.78	1.54	1.50
25	9	306	CLA	C3B-C4B	2.78	1.49	1.42
24	1	309	CHL	C3B-C4B	2.78	1.49	1.42
24	1	317	CHL	C4D-CHA	2.78	1.48	1.38
24	G	309	CHL	C4D-CHA	2.78	1.48	1.38
25	Y	313	CLA	C4B-NB	2.78	1.41	1.37
25	b	604	CLA	C4B-NB	2.78	1.41	1.37
25	g	307	CLA	C3B-C4B	2.78	1.49	1.42
25	5	314	CLA	C3B-C4B	2.78	1.49	1.42
24	g	309	CHL	C4D-CHA	2.78	1.48	1.38
25	2	308	CLA	C3B-C4B	2.78	1.49	1.42
25	4	306	CLA	C3B-C4B	2.78	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	315	CHL	C4D-CHA	2.77	1.48	1.38
25	B	613	CLA	C4B-NB	2.77	1.41	1.37
25	c	603	CLA	C4B-NB	2.77	1.41	1.37
24	8	308	CHL	MG-NA	-2.77	1.99	2.06
24	4	317	CHL	C4D-CHA	2.77	1.48	1.38
25	q	315	CLA	C3B-C4B	2.77	1.49	1.42
25	2	314	CLA	C3B-C4B	2.77	1.49	1.42
24	n	305	CHL	MG-NA	-2.77	1.99	2.06
24	y	306	CHL	MG-NA	-2.77	1.99	2.06
24	Y	311	CHL	MG-NA	-2.77	1.99	2.06
24	y	312	CHL	MG-NA	-2.77	1.99	2.06
25	r	311	CLA	C3B-C4B	2.77	1.49	1.42
31	s	415	8CT	C07-C02	-2.77	1.45	1.51
25	B	615	CLA	C3B-C4B	2.77	1.49	1.42
24	n	317	CHL	C4D-CHA	2.77	1.48	1.38
25	C	603	CLA	C4B-NB	2.77	1.41	1.37
24	u	309	CHL	C4D-CHA	2.77	1.48	1.38
25	d	404	CLA	C4B-NB	2.77	1.41	1.37
25	n	315	CLA	C3B-C4B	2.77	1.49	1.42
24	N	305	CHL	MG-NA	-2.76	1.99	2.06
24	4	311	CHL	C3B-C4B	2.76	1.49	1.42
25	Y	306	CLA	C4B-NB	2.76	1.41	1.37
24	1	311	CHL	MG-NA	-2.76	1.99	2.06
25	S	616	CLA	C3B-C4B	2.76	1.49	1.42
35	D	403	PHO	CMC-C2C	-2.76	1.46	1.50
25	B	605	CLA	C3B-C4B	2.76	1.49	1.42
24	p	309	CHL	C4D-CHA	2.76	1.48	1.38
31	S	614	8CT	C07-C02	-2.76	1.45	1.51
24	6	308	CHL	C4D-CHA	2.76	1.48	1.38
25	G	316	CLA	C3B-C4B	2.76	1.49	1.42
24	N	311	CHL	MG-NA	-2.75	1.99	2.06
25	9	307	CLA	C3B-C4B	2.75	1.49	1.42
25	7	308	CLA	C3B-C4B	2.75	1.49	1.42
24	9	317	CHL	C4D-CHA	2.75	1.48	1.38
24	1	311	CHL	C3B-C4B	2.75	1.49	1.42
25	8	314	CLA	C3B-C4B	2.75	1.49	1.42
24	4	304	CHL	C4D-CHA	2.75	1.48	1.38
24	1	304	CHL	C4D-CHA	2.75	1.48	1.38
25	b	610	CLA	C3B-C4B	2.75	1.49	1.42
24	u	318	CHL	C4D-CHA	2.75	1.48	1.38
25	b	613	CLA	C3B-C4B	2.74	1.49	1.42
24	3	308	CHL	C4D-CHA	2.74	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	316	CLA	C3B-C4B	2.74	1.49	1.42
31	a	608	8CT	C30-C29	2.74	1.54	1.50
25	C	611	CLA	C4B-NB	2.74	1.41	1.37
24	9	317	CHL	C3B-C4B	2.74	1.49	1.42
25	C	605	CLA	C4B-NB	2.74	1.41	1.37
24	g	306	CHL	MG-NA	-2.74	1.99	2.06
31	C	615	8CT	C07-C02	-2.74	1.45	1.51
25	2	316	CLA	C3B-C4B	2.74	1.49	1.42
25	q	313	CLA	C3B-C4B	2.74	1.49	1.42
25	c	609	CLA	C4B-NB	2.73	1.41	1.37
31	c	614	8CT	C35-C30	2.73	1.64	1.56
24	q	316	CHL	C4D-CHA	2.73	1.48	1.38
31	C	614	8CT	C35-C30	2.73	1.64	1.56
25	1	307	CLA	C3B-C4B	2.73	1.49	1.42
25	R	611	CLA	C3B-C4B	2.73	1.49	1.42
25	B	610	CLA	C3B-C4B	2.73	1.49	1.42
25	b	615	CLA	C3B-C4B	2.73	1.49	1.42
25	8	312	CLA	C3B-C4B	2.73	1.49	1.42
25	3	306	CLA	C3B-C4B	2.73	1.49	1.42
25	c	612	CLA	C4B-NB	2.73	1.41	1.37
35	d	403	PHO	CMC-C2C	-2.73	1.46	1.50
24	4	308	CHL	C4D-CHA	2.73	1.48	1.38
25	N	315	CLA	C3B-C4B	2.73	1.49	1.42
25	p	314	CLA	C3B-C4B	2.73	1.49	1.42
25	9	307	CLA	C1B-C2B	2.72	1.49	1.43
25	B	613	CLA	C3B-C4B	2.72	1.49	1.42
25	u	316	CLA	C1B-C2B	2.72	1.49	1.43
24	u	318	CHL	C3B-C4B	2.72	1.49	1.42
24	n	311	CHL	MG-NA	-2.72	1.99	2.06
24	u	309	CHL	C3B-C4B	2.72	1.49	1.42
24	N	317	CHL	C3B-C4B	2.72	1.49	1.42
25	C	611	CLA	C3B-C4B	2.72	1.49	1.42
24	n	317	CHL	C3B-C4B	2.72	1.49	1.42
25	c	611	CLA	C3B-C4B	2.72	1.49	1.42
24	Y	310	CHL	MG-NA	-2.72	1.99	2.06
24	y	311	CHL	MG-NA	-2.72	1.99	2.06
25	5	316	CLA	C3B-C4B	2.72	1.49	1.42
25	q	312	CLA	C3B-C4B	2.72	1.49	1.42
25	q	314	CLA	C3B-C4B	2.72	1.49	1.42
25	b	605	CLA	C3B-C4B	2.72	1.49	1.42
24	1	308	CHL	C4D-CHA	2.72	1.48	1.38
25	r	313	CLA	C3B-C4B	2.72	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	309	CHL	C3B-C4B	2.72	1.49	1.42
25	N	306	CLA	C3B-C4B	2.71	1.49	1.42
25	c	616	CLA	C4B-NB	2.71	1.41	1.37
31	D	410	8CT	C07-C02	-2.71	1.45	1.51
31	S	615	8CT	C07-C02	-2.71	1.45	1.51
24	u	312	CHL	C4D-CHA	2.71	1.48	1.38
25	1	316	CLA	C1B-C2B	2.71	1.49	1.43
31	c	615	8CT	C07-C02	-2.71	1.45	1.51
24	5	310	CHL	MG-NA	-2.71	1.99	2.06
35	A	606	PHO	CMC-C2C	-2.70	1.46	1.50
24	1	317	CHL	C3B-C4B	2.70	1.49	1.42
25	C	609	CLA	C4B-NB	2.70	1.41	1.37
31	b	617	8CT	C30-C29	2.70	1.54	1.50
24	G	309	CHL	C3B-C4B	2.70	1.49	1.42
24	5	318	CHL	C4D-CHA	2.70	1.48	1.38
35	a	606	PHO	CMB-C2B	-2.70	1.46	1.51
25	y	314	CLA	C3B-C4B	2.70	1.49	1.42
24	9	311	CHL	C4D-CHA	2.70	1.48	1.38
25	C	616	CLA	C4B-NB	2.70	1.41	1.37
25	4	307	CLA	C3B-C4B	2.70	1.49	1.42
25	b	606	CLA	C4B-NB	2.70	1.41	1.37
24	9	308	CHL	C3B-C4B	2.70	1.49	1.42
31	A	608	8CT	C30-C29	2.70	1.54	1.50
25	6	306	CLA	C3B-C4B	2.70	1.49	1.42
24	n	304	CHL	C4D-CHA	2.70	1.48	1.38
25	c	611	CLA	C4B-NB	2.69	1.41	1.37
25	9	315	CLA	C1B-C2B	2.69	1.49	1.43
25	Y	313	CLA	C3B-C4B	2.69	1.49	1.42
25	n	306	CLA	C3B-C4B	2.69	1.49	1.42
25	b	607	CLA	C3B-C4B	2.69	1.49	1.42
25	r	312	CLA	C3B-C4B	2.69	1.49	1.42
25	D	404	CLA	C4B-NB	2.69	1.41	1.37
31	d	410	8CT	C07-C02	-2.69	1.45	1.51
25	5	317	CLA	C3B-C4B	2.69	1.49	1.42
24	p	310	CHL	C3B-C4B	2.69	1.49	1.42
35	A	606	PHO	CMD-C2D	-2.69	1.46	1.51
25	r	313	CLA	C1B-C2B	2.69	1.49	1.43
24	y	310	CHL	C3B-C4B	2.69	1.49	1.42
24	6	311	CHL	MG-NA	-2.69	1.99	2.06
35	a	606	PHO	CMD-C2D	-2.69	1.46	1.51
24	2	318	CHL	C4D-CHA	2.69	1.48	1.38
24	g	312	CHL	C3B-C4B	2.69	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	u	317	CLA	C1B-C2B	2.69	1.49	1.43
24	5	309	CHL	C4D-CHA	2.68	1.47	1.38
31	B	617	8CT	C07-C02	-2.68	1.45	1.51
24	r	308	CHL	MG-NA	-2.68	1.99	2.06
31	b	617	8CT	C07-C02	-2.68	1.45	1.51
25	B	611	CLA	CMB-C2B	-2.68	1.45	1.50
24	2	309	CHL	C4D-CHA	2.68	1.47	1.38
25	B	606	CLA	C4B-NB	2.68	1.41	1.37
25	7	314	CLA	C3B-C4B	2.68	1.49	1.42
24	1	310	CHL	C3B-C4B	2.68	1.49	1.42
24	4	305	CHL	C3B-C4B	2.68	1.49	1.42
25	b	611	CLA	CMB-C2B	-2.68	1.45	1.50
25	8	306	CLA	C3B-C4B	2.68	1.49	1.42
25	R	604	CLA	C3B-C4B	2.68	1.49	1.42
25	9	306	CLA	C1B-C2B	2.68	1.49	1.43
25	2	317	CLA	C3B-C4B	2.68	1.49	1.42
25	8	311	CLA	C3B-C4B	2.68	1.49	1.42
24	N	304	CHL	C4D-CHA	2.67	1.47	1.38
24	4	317	CHL	C3B-C4B	2.67	1.49	1.42
25	c	605	CLA	C4B-NB	2.67	1.41	1.37
24	2	312	CHL	MG-NA	-2.67	1.99	2.06
25	9	316	CLA	C1B-C2B	2.67	1.49	1.43
24	u	306	CHL	C3B-C4B	2.67	1.49	1.42
25	C	612	CLA	C4B-NB	2.67	1.41	1.37
25	u	308	CLA	C1B-C2B	2.67	1.49	1.43
35	a	606	PHO	C4D-ND	-2.67	1.34	1.38
25	6	313	CLA	C1B-C2B	2.67	1.49	1.43
24	R	601	CHL	C3B-C4B	2.67	1.49	1.42
25	n	315	CLA	C1B-C2B	2.67	1.49	1.43
24	8	310	CHL	C1B-NB	-2.67	1.34	1.37
24	q	310	CHL	MG-NA	-2.67	1.99	2.06
25	8	313	CLA	C3B-C4B	2.67	1.49	1.42
24	u	305	CHL	C4D-CHA	2.67	1.47	1.38
25	A	605	CLA	C4B-NB	2.67	1.41	1.37
25	4	316	CLA	C1B-C2B	2.67	1.49	1.43
24	8	309	CHL	MG-NA	-2.67	1.99	2.06
25	n	316	CLA	C1B-C2B	2.67	1.49	1.43
24	p	306	CHL	MG-NA	-2.66	1.99	2.06
24	n	308	CHL	C4D-CHA	2.66	1.47	1.38
25	u	315	CLA	C1B-C2B	2.66	1.49	1.43
25	B	608	CLA	C3B-C4B	2.66	1.49	1.42
25	b	608	CLA	C3B-C4B	2.66	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	315	CLA	C3B-C4B	2.66	1.49	1.42
25	N	315	CLA	C1B-C2B	2.66	1.49	1.43
25	4	315	CLA	C1B-C2B	2.66	1.49	1.43
24	9	311	CHL	C3B-C4B	2.66	1.49	1.42
24	R	607	CHL	MG-NA	-2.66	2.00	2.06
31	s	416	8CT	C07-C02	-2.66	1.45	1.51
25	c	612	CLA	C3B-C4B	2.66	1.49	1.42
24	g	309	CHL	C3B-C4B	2.66	1.49	1.42
25	b	602	CLA	C3B-C4B	2.66	1.49	1.42
25	B	603	CLA	C4B-NB	2.66	1.41	1.37
25	q	306	CLA	C3B-C4B	2.66	1.49	1.42
25	9	314	CLA	C1B-C2B	2.66	1.49	1.43
25	Y	316	CLA	C3B-C4B	2.66	1.49	1.42
24	r	306	CHL	C3B-C4B	2.66	1.49	1.42
24	r	302	CHL	C4D-CHA	2.66	1.47	1.38
25	4	314	CLA	C1B-C2B	2.66	1.49	1.43
24	7	310	CHL	C3B-C4B	2.65	1.49	1.42
25	B	607	CLA	C3B-C4B	2.65	1.49	1.42
25	B	611	CLA	C3B-C4B	2.65	1.49	1.42
25	u	307	CLA	C1B-C2B	2.65	1.49	1.43
25	N	314	CLA	C1B-C2B	2.65	1.49	1.43
25	n	306	CLA	C1B-C2B	2.65	1.49	1.43
25	y	317	CLA	C3B-C4B	2.65	1.49	1.42
25	2	307	CLA	C3B-C4B	2.65	1.49	1.42
25	B	612	CLA	MG-NB	-2.65	2.00	2.05
25	b	603	CLA	C4B-NB	2.65	1.41	1.37
25	1	315	CLA	C1B-C2B	2.65	1.49	1.43
24	4	308	CHL	C3B-C4B	2.65	1.49	1.42
24	4	310	CHL	C3B-C4B	2.65	1.49	1.42
25	q	314	CLA	C1B-C2B	2.65	1.49	1.43
35	a	606	PHO	CAC-C3C	-2.65	1.46	1.51
25	5	307	CLA	C3B-C4B	2.65	1.49	1.42
25	b	612	CLA	MG-NB	-2.65	2.00	2.05
24	R	601	CHL	C4D-CHA	2.65	1.47	1.38
24	r	302	CHL	C3B-C4B	2.64	1.49	1.42
24	8	304	CHL	C1B-NB	-2.64	1.34	1.37
25	8	313	CLA	C1B-C2B	2.64	1.49	1.43
25	n	314	CLA	C1B-C2B	2.64	1.49	1.43
24	G	312	CHL	C3B-C4B	2.64	1.49	1.42
25	3	313	CLA	C1B-C2B	2.64	1.49	1.43
24	7	306	CHL	MG-NA	-2.64	2.00	2.06
24	u	312	CHL	C3B-C4B	2.64	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	612	CLA	C1B-C2B	2.64	1.49	1.43
24	8	304	CHL	C3B-C4B	2.64	1.48	1.42
35	A	606	PHO	CAC-C3C	-2.64	1.46	1.51
25	R	613	CLA	C1B-C2B	2.64	1.49	1.43
24	6	308	CHL	C3B-C4B	2.64	1.48	1.42
25	s	412	CLA	C3B-C4B	2.64	1.48	1.42
24	y	310	CHL	MG-NA	-2.64	2.00	2.06
24	1	304	CHL	C3B-C4B	2.64	1.48	1.42
24	5	312	CHL	MG-NA	-2.64	2.00	2.06
25	p	316	CLA	C3B-C4B	2.64	1.48	1.42
25	6	306	CLA	C1B-C2B	2.64	1.49	1.43
35	A	606	PHO	CMB-C2B	-2.64	1.46	1.51
24	s	407	CHL	C3B-C4B	2.64	1.48	1.42
25	u	314	CLA	C1B-C2B	2.63	1.49	1.43
25	a	610	CLA	C1B-C2B	2.63	1.49	1.43
25	3	315	CLA	C1B-C2B	2.63	1.49	1.43
24	N	304	CHL	C3B-C4B	2.63	1.48	1.42
25	y	308	CLA	C3B-C4B	2.63	1.48	1.42
25	G	316	CLA	C1B-C2B	2.63	1.49	1.43
24	9	304	CHL	C4D-CHA	2.63	1.47	1.38
24	7	318	CHL	C4D-CHA	2.63	1.47	1.38
24	n	311	CHL	C3B-C4B	2.63	1.48	1.42
35	A	606	PHO	C4D-ND	-2.63	1.34	1.38
24	u	305	CHL	C3B-C4B	2.63	1.48	1.42
25	R	603	CLA	C3B-C4B	2.63	1.48	1.42
25	r	314	CLA	C1B-C2B	2.63	1.49	1.43
25	p	315	CLA	C3B-C4B	2.63	1.48	1.42
25	4	307	CLA	C1B-C2B	2.63	1.49	1.43
25	c	603	CLA	C3B-C4B	2.63	1.48	1.42
25	s	404	CLA	C1B-C2B	2.63	1.49	1.43
25	B	602	CLA	C3B-C4B	2.63	1.48	1.42
24	p	318	CHL	C4D-CHA	2.63	1.47	1.38
25	y	316	CLA	C4B-NB	2.63	1.41	1.37
25	b	601	CLA	C3B-C4B	2.63	1.48	1.42
25	S	611	CLA	C3B-C4B	2.63	1.48	1.42
24	1	308	CHL	C3B-C4B	2.63	1.48	1.42
24	6	310	CHL	C4D-CHA	2.63	1.47	1.38
24	8	303	CHL	C4D-CHA	2.63	1.47	1.38
25	1	314	CLA	C1B-C2B	2.63	1.49	1.43
24	4	304	CHL	C3B-C4B	2.62	1.48	1.42
35	d	403	PHO	CMD-C2D	-2.62	1.46	1.51
24	p	318	CHL	C3B-C4B	2.62	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	608	CLA	C4B-NB	2.62	1.41	1.37
24	1	305	CHL	C3B-C4B	2.62	1.48	1.42
25	7	316	CLA	C3B-C4B	2.62	1.48	1.42
25	S	603	CLA	C3B-C4B	2.62	1.48	1.42
25	B	601	CLA	C3B-C4B	2.62	1.48	1.42
25	c	616	CLA	MG-NB	-2.62	2.00	2.05
25	A	610	CLA	C1B-C2B	2.62	1.49	1.43
24	3	308	CHL	C3B-C4B	2.62	1.48	1.42
25	3	306	CLA	C1B-C2B	2.62	1.49	1.43
25	p	308	CLA	C1B-C2B	2.62	1.49	1.43
24	q	304	CHL	C3B-C4B	2.62	1.48	1.42
24	7	309	CHL	C3B-C4B	2.62	1.48	1.42
25	6	307	CLA	C1B-C2B	2.62	1.49	1.43
24	7	318	CHL	C3B-C4B	2.62	1.48	1.42
25	C	610	CLA	C4B-NB	2.62	1.41	1.37
25	g	316	CLA	C1B-C2B	2.62	1.49	1.43
25	N	316	CLA	C1B-C2B	2.62	1.49	1.43
25	A	603	CLA	C3B-C4B	2.62	1.48	1.42
25	a	603	CLA	C3B-C4B	2.62	1.48	1.42
24	8	315	CHL	C3B-C4B	2.62	1.48	1.42
25	7	307	CLA	C3B-C4B	2.62	1.48	1.42
25	9	313	CLA	C1B-C2B	2.62	1.49	1.43
25	b	603	CLA	MG-NB	-2.62	2.00	2.05
25	c	606	CLA	C4B-NB	2.62	1.41	1.37
25	3	307	CLA	C1B-C2B	2.62	1.49	1.43
25	B	612	CLA	C4B-NB	2.62	1.41	1.37
35	D	403	PHO	CMD-C2D	-2.61	1.46	1.51
24	9	310	CHL	C3B-C4B	2.61	1.48	1.42
25	1	307	CLA	C1B-C2B	2.61	1.49	1.43
39	D	406	PL9	C52-C5	-2.61	1.45	1.50
26	q	302	0IE	C13-C12	-2.61	1.40	1.45
24	S	606	CHL	C3B-C4B	2.61	1.48	1.42
25	b	611	CLA	C3B-C4B	2.61	1.48	1.42
24	q	303	CHL	C4D-CHA	2.61	1.47	1.38
25	b	614	CLA	C3B-C4B	2.61	1.48	1.42
25	6	314	CLA	C1B-C2B	2.61	1.49	1.43
25	B	603	CLA	MG-NB	-2.61	2.00	2.05
25	Y	307	CLA	C3B-C4B	2.61	1.48	1.42
25	C	612	CLA	C3B-C4B	2.61	1.48	1.42
25	1	306	CLA	C1B-C2B	2.61	1.49	1.43
24	Y	309	CHL	MG-NA	-2.61	2.00	2.06
25	r	304	CLA	C3B-C4B	2.61	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	304	CHL	MG-NA	-2.61	2.00	2.06
24	g	310	CHL	C3B-C4B	2.61	1.48	1.42
25	C	608	CLA	C4B-NB	2.61	1.41	1.37
25	y	307	CLA	C3B-C4B	2.61	1.48	1.42
24	G	310	CHL	C3B-C4B	2.61	1.48	1.42
25	7	308	CLA	C1B-C2B	2.61	1.49	1.43
25	C	606	CLA	C4B-NB	2.61	1.41	1.37
24	6	304	CHL	C4D-CHA	2.61	1.47	1.38
24	n	304	CHL	C3B-C4B	2.60	1.48	1.42
25	N	306	CLA	C1B-C2B	2.60	1.49	1.43
25	6	315	CLA	C1B-C2B	2.60	1.49	1.43
24	n	310	CHL	C4D-CHA	2.60	1.47	1.38
25	B	614	CLA	C3B-C4B	2.60	1.48	1.42
25	d	405	CLA	C3B-C4B	2.60	1.48	1.42
24	9	310	CHL	C4D-CHA	2.60	1.47	1.38
24	p	311	CHL	C3B-C4B	2.60	1.48	1.42
24	G	306	CHL	C3B-C4B	2.60	1.48	1.42
25	s	404	CLA	C3B-C4B	2.60	1.48	1.42
25	5	317	CLA	C1B-C2B	2.60	1.49	1.43
24	y	305	CHL	MG-NA	-2.60	2.00	2.06
24	G	312	CHL	C4D-CHA	2.60	1.47	1.38
25	p	317	CLA	C1B-C2B	2.60	1.49	1.43
25	p	307	CLA	C3B-C4B	2.60	1.48	1.42
24	3	317	CHL	C4D-CHA	2.60	1.47	1.38
25	r	305	CLA	C3B-C4B	2.60	1.48	1.42
25	c	607	CLA	C4B-NB	2.60	1.41	1.37
39	d	406	PL9	C52-C5	-2.60	1.45	1.50
25	c	604	CLA	C3B-C4B	2.60	1.48	1.42
24	r	307	CHL	C3B-C4B	2.60	1.48	1.42
24	u	310	CHL	C4D-CHA	2.60	1.47	1.38
24	n	310	CHL	C3B-C4B	2.60	1.48	1.42
25	g	315	CLA	C1B-C2B	2.59	1.49	1.43
24	p	309	CHL	C3B-C4B	2.59	1.48	1.42
25	Y	306	CLA	C3B-C4B	2.59	1.48	1.42
24	3	310	CHL	C4D-CHA	2.59	1.47	1.38
24	G	313	CHL	C3B-C4B	2.59	1.48	1.42
25	G	315	CLA	C1B-C2B	2.59	1.49	1.43
25	q	315	CLA	C1B-C2B	2.59	1.49	1.43
24	u	311	CHL	C4D-CHA	2.59	1.47	1.38
25	C	616	CLA	MG-NB	-2.59	2.00	2.05
24	N	311	CHL	C3B-C4B	2.59	1.48	1.42
25	a	605	CLA	C4B-NB	2.59	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	317	CHL	C1B-C2B	2.59	1.49	1.43
25	C	603	CLA	C3B-C4B	2.59	1.48	1.42
25	2	316	CLA	C1B-C2B	2.59	1.49	1.43
25	G	314	CLA	C1B-C2B	2.59	1.49	1.43
24	g	305	CHL	C4D-CHA	2.59	1.47	1.38
31	c	613	8CT	C30-C29	2.59	1.54	1.50
24	Y	308	CHL	C4D-CHA	2.59	1.47	1.38
25	6	316	CLA	C1B-C2B	2.59	1.49	1.43
24	g	311	CHL	C3B-C4B	2.59	1.48	1.42
25	C	604	CLA	C3B-C4B	2.59	1.48	1.42
24	g	306	CHL	C3B-C4B	2.59	1.48	1.42
25	C	608	CLA	CMB-C2B	-2.59	1.45	1.50
25	8	314	CLA	C1B-C2B	2.59	1.49	1.43
31	B	617	8CT	C30-C29	2.59	1.54	1.50
25	n	313	CLA	C1B-C2B	2.59	1.49	1.43
25	c	610	CLA	C4B-NB	2.59	1.41	1.37
24	6	317	CHL	C4D-CHA	2.59	1.47	1.38
24	G	305	CHL	C4D-CHA	2.58	1.47	1.38
26	y	302	0IE	C6-C7	-2.58	1.40	1.45
24	N	310	CHL	C3B-C4B	2.58	1.48	1.42
24	g	318	CHL	C4D-CHA	2.58	1.47	1.38
24	y	309	CHL	C4D-CHA	2.58	1.47	1.38
24	7	305	CHL	MG-NA	-2.58	2.00	2.06
25	C	608	CLA	C3B-C4B	2.58	1.48	1.42
24	N	309	CHL	MG-NA	-2.58	2.00	2.06
25	4	306	CLA	C1B-C2B	2.58	1.49	1.43
25	s	405	CLA	C1B-C2B	2.58	1.49	1.43
24	3	312	CHL	C4D-CHA	2.58	1.47	1.38
25	C	605	CLA	C3B-C4B	2.58	1.48	1.42
25	D	405	CLA	C3B-C4B	2.58	1.48	1.42
25	S	604	CLA	C1B-C2B	2.58	1.49	1.43
24	q	307	CHL	C4D-CHA	2.58	1.47	1.38
24	q	316	CHL	C3B-C4B	2.58	1.48	1.42
24	N	310	CHL	C4D-CHA	2.58	1.47	1.38
24	g	311	CHL	C4D-CHA	2.58	1.47	1.38
24	2	309	CHL	C3B-C4B	2.58	1.48	1.42
25	c	605	CLA	C3B-C4B	2.58	1.48	1.42
25	4	313	CLA	C1B-C2B	2.58	1.49	1.43
24	u	311	CHL	C3B-C4B	2.58	1.48	1.42
24	Y	305	CHL	C1B-NB	-2.58	1.34	1.37
24	q	310	CHL	C1B-NB	-2.58	1.34	1.37
24	3	309	CHL	C3B-C4B	2.58	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	308	CLA	C1B-C2B	2.58	1.49	1.43
25	7	317	CLA	C1B-C2B	2.58	1.49	1.43
24	3	317	CHL	C3B-C4B	2.58	1.48	1.42
24	g	310	CHL	C4D-CHA	2.58	1.47	1.38
24	y	306	CHL	C1B-NB	-2.58	1.34	1.37
25	Y	315	CLA	C4B-NB	2.58	1.41	1.37
25	g	314	CLA	C1B-C2B	2.58	1.49	1.43
24	4	317	CHL	C1B-C2B	2.58	1.49	1.43
24	6	312	CHL	C3B-C4B	2.58	1.48	1.42
24	p	305	CHL	MG-NA	-2.58	2.00	2.06
25	5	316	CLA	C1B-C2B	2.57	1.49	1.43
25	s	411	CLA	C3B-C4B	2.57	1.48	1.42
24	u	309	CHL	C1B-C2B	2.57	1.49	1.43
24	9	305	CHL	C3B-C4B	2.57	1.48	1.42
26	8	302	0IE	C13-C12	-2.57	1.40	1.45
25	7	307	CLA	C1B-C2B	2.57	1.49	1.43
25	b	612	CLA	C3B-C4B	2.57	1.48	1.42
24	9	312	CHL	C4D-CHA	2.57	1.47	1.38
24	u	313	CHL	C4D-CHA	2.57	1.47	1.38
24	3	310	CHL	C3B-C4B	2.57	1.48	1.42
30	Y	318	LHG	O8-C6	-2.57	1.39	1.45
24	9	311	CHL	C1B-C2B	2.57	1.49	1.43
24	8	307	CHL	C4D-CHA	2.57	1.47	1.38
24	q	311	CHL	C1B-NB	-2.57	1.34	1.37
25	r	312	CLA	C1B-C2B	2.57	1.49	1.43
24	2	305	CHL	C3B-C4B	2.57	1.48	1.42
25	C	602	CLA	C4B-NB	2.57	1.40	1.37
25	c	602	CLA	C4B-NB	2.57	1.40	1.37
26	Y	303	0IE	C13-C12	-2.57	1.40	1.45
24	R	606	CHL	C3B-C4B	2.57	1.48	1.42
25	s	413	CLA	C3B-C4B	2.57	1.48	1.42
25	C	610	CLA	C3B-C4B	2.57	1.48	1.42
24	G	310	CHL	C4D-CHA	2.57	1.47	1.38
24	7	311	CHL	C3B-C4B	2.57	1.48	1.42
24	q	308	CHL	C1B-NB	-2.57	1.34	1.37
24	G	312	CHL	C1B-C2B	2.57	1.49	1.43
25	S	603	CLA	C1B-C2B	2.57	1.49	1.43
24	5	313	CHL	C3B-C4B	2.57	1.48	1.42
25	A	607	CLA	C4B-NB	2.57	1.40	1.37
35	D	403	PHO	CMB-C2B	-2.57	1.46	1.51
24	2	305	CHL	C4D-CHA	2.57	1.47	1.38
23	f	201	HEM	FE-NC	2.57	2.03	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	305	CHL	C3B-C4B	2.56	1.48	1.42
35	d	403	PHO	CMB-C2B	-2.56	1.46	1.51
25	D	404	CLA	C3B-C4B	2.56	1.48	1.42
25	d	404	CLA	C3B-C4B	2.56	1.48	1.42
24	6	317	CHL	C3B-C4B	2.56	1.48	1.42
24	7	312	CHL	MG-NA	-2.56	2.00	2.06
24	q	304	CHL	C1B-NB	-2.56	1.34	1.37
25	8	305	CLA	C1B-C2B	2.56	1.49	1.43
25	R	603	CLA	C1B-C2B	2.56	1.49	1.43
24	6	312	CHL	C4D-CHA	2.56	1.47	1.38
24	g	313	CHL	C4D-CHA	2.56	1.47	1.38
24	8	308	CHL	C3B-C4B	2.56	1.48	1.42
24	5	305	CHL	C3B-C4B	2.56	1.48	1.42
24	9	304	CHL	C1B-C2B	2.56	1.49	1.43
24	6	309	CHL	C4D-CHA	2.56	1.47	1.38
26	y	302	0IE	C13-C12	-2.56	1.40	1.45
26	y	302	0IE	C17-C16	-2.56	1.40	1.45
31	C	613	8CT	C30-C29	2.56	1.54	1.50
24	5	309	CHL	C3B-C4B	2.56	1.48	1.42
26	8	302	0IE	C17-C16	-2.56	1.40	1.45
24	9	312	CHL	C3B-C4B	2.56	1.48	1.42
24	6	309	CHL	C3B-C4B	2.56	1.48	1.42
30	D	408	LHG	O8-C6	-2.56	1.39	1.45
25	c	606	CLA	C3B-C4B	2.56	1.48	1.42
26	y	303	0IE	C13-C12	-2.56	1.40	1.45
24	8	309	CHL	C1B-NB	-2.56	1.34	1.37
25	8	312	CLA	C1B-C2B	2.56	1.49	1.43
24	7	309	CHL	C1B-C2B	2.56	1.49	1.43
25	G	308	CLA	C1B-C2B	2.56	1.49	1.43
24	g	312	CHL	C4D-CHA	2.56	1.47	1.38
25	R	611	CLA	C1B-C2B	2.56	1.49	1.43
24	R	605	CHL	MG-NA	-2.56	2.00	2.06
24	g	313	CHL	C3B-C4B	2.56	1.48	1.42
24	3	311	CHL	C4D-CHA	2.56	1.47	1.38
24	9	308	CHL	C1B-C2B	2.56	1.49	1.43
25	2	317	CLA	C1B-C2B	2.56	1.49	1.43
24	8	308	CHL	C1B-NB	-2.56	1.34	1.37
31	c	613	8CT	C35-C30	2.56	1.63	1.56
25	c	608	CLA	C3B-C4B	2.56	1.48	1.42
25	b	612	CLA	C4B-NB	2.56	1.40	1.37
25	C	606	CLA	C3B-C4B	2.56	1.48	1.42
25	N	313	CLA	C1B-C2B	2.55	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	309	CHL	C1B-C2B	2.55	1.49	1.43
25	C	605	CLA	CMD-C2D	-2.55	1.45	1.50
25	S	616	CLA	C1B-C2B	2.55	1.49	1.43
24	u	313	CHL	C3B-C4B	2.55	1.48	1.42
24	3	309	CHL	C4D-CHA	2.55	1.47	1.38
24	Y	304	CHL	C1C-NC	-2.55	1.34	1.37
25	3	316	CLA	C1B-C2B	2.55	1.49	1.43
25	S	612	CLA	C3B-C4B	2.55	1.48	1.42
25	8	305	CLA	C3B-C4B	2.55	1.48	1.42
25	1	313	CLA	C1B-C2B	2.55	1.49	1.43
25	p	316	CLA	C1B-C2B	2.55	1.49	1.43
25	7	316	CLA	C1B-C2B	2.55	1.49	1.43
25	S	610	CLA	C3B-C4B	2.55	1.48	1.42
24	p	309	CHL	C1B-C2B	2.55	1.49	1.43
24	9	309	CHL	C4D-CHA	2.55	1.47	1.38
24	6	310	CHL	C3B-C4B	2.55	1.48	1.42
25	B	612	CLA	C3B-C4B	2.55	1.48	1.42
24	G	311	CHL	C4D-CHA	2.55	1.47	1.38
24	G	313	CHL	C4D-CHA	2.55	1.47	1.38
24	g	312	CHL	C1B-C2B	2.55	1.49	1.43
25	c	608	CLA	CMB-C2B	-2.55	1.45	1.50
24	n	308	CHL	C3B-C4B	2.55	1.48	1.42
24	G	318	CHL	C4D-CHA	2.55	1.47	1.38
35	d	403	PHO	CAC-C3C	-2.55	1.47	1.51
25	s	410	CLA	C1B-C2B	2.55	1.49	1.43
24	G	311	CHL	C3B-C4B	2.55	1.48	1.42
30	D	407	LHG	O8-C6	-2.55	1.39	1.45
25	S	604	CLA	C3B-C4B	2.55	1.48	1.42
25	C	607	CLA	C4B-NB	2.55	1.40	1.37
25	c	610	CLA	C3B-C4B	2.55	1.48	1.42
31	C	613	8CT	C35-C30	2.55	1.63	1.56
25	3	314	CLA	C1B-C2B	2.55	1.49	1.43
25	s	417	CLA	C1B-C2B	2.55	1.49	1.43
25	r	304	CLA	C1B-C2B	2.55	1.49	1.43
25	C	606	CLA	MG-NB	-2.55	2.00	2.05
24	q	316	CHL	C1B-C2B	2.55	1.49	1.43
25	c	601	CLA	MG-NB	-2.55	2.00	2.05
24	5	305	CHL	C4D-CHA	2.55	1.47	1.38
25	n	307	CLA	C1B-C2B	2.55	1.49	1.43
25	q	305	CLA	C1B-C2B	2.55	1.49	1.43
24	q	309	CHL	C1B-NB	-2.55	1.34	1.37
25	s	413	CLA	C1B-C2B	2.55	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	609	CLA	C1B-C2B	2.55	1.49	1.43
24	n	305	CHL	C3B-C4B	2.54	1.48	1.42
24	9	304	CHL	C3B-C4B	2.54	1.48	1.42
24	q	308	CHL	C3B-C4B	2.54	1.48	1.42
24	6	312	CHL	C1B-C2B	2.54	1.49	1.43
24	y	313	CHL	C1B-NB	-2.54	1.34	1.37
24	G	305	CHL	C3B-C4B	2.54	1.48	1.42
24	3	304	CHL	C4D-CHA	2.54	1.47	1.38
25	R	609	CLA	C1B-C2B	2.54	1.49	1.43
25	q	313	CLA	C1B-C2B	2.54	1.49	1.43
25	b	606	CLA	C3B-C4B	2.54	1.48	1.42
30	d	407	LHG	O8-C6	-2.54	1.39	1.45
30	D	407	LHG	O7-C5	-2.54	1.40	1.46
25	a	607	CLA	C3B-C4B	2.54	1.48	1.42
26	Y	302	0IE	C6-C7	-2.54	1.40	1.45
24	N	308	CHL	C4D-CHA	2.54	1.47	1.38
24	u	305	CHL	C1B-C2B	2.54	1.49	1.43
25	c	601	CLA	C4B-NB	2.54	1.40	1.37
25	A	605	CLA	MG-NB	-2.54	2.00	2.05
25	B	616	CLA	C1B-C2B	2.54	1.49	1.43
24	G	318	CHL	C3B-C4B	2.54	1.48	1.42
25	c	605	CLA	CMD-C2D	-2.54	1.45	1.50
24	4	304	CHL	C1B-C2B	2.54	1.49	1.43
24	u	312	CHL	C1B-C2B	2.54	1.49	1.43
24	5	310	CHL	C4D-CHA	2.54	1.47	1.38
24	7	306	CHL	C3B-C4B	2.54	1.48	1.42
26	5	302	0IE	C6-C7	-2.54	1.40	1.45
24	2	313	CHL	C3B-C4B	2.53	1.48	1.42
24	p	306	CHL	C3B-C4B	2.53	1.48	1.42
26	Y	302	0IE	C13-C12	-2.53	1.40	1.45
31	S	615	8CT	C25-C26	2.53	1.39	1.35
25	B	606	CLA	C3B-C4B	2.53	1.48	1.42
25	b	616	CLA	C1B-C2B	2.53	1.49	1.43
24	9	317	CHL	C4C-C3C	2.53	1.49	1.45
24	n	317	CHL	C1B-C2B	2.53	1.49	1.43
25	c	606	CLA	CMB-C2B	-2.53	1.45	1.50
31	s	416	8CT	C25-C26	2.53	1.39	1.35
24	3	312	CHL	C3B-C4B	2.53	1.48	1.42
24	4	309	CHL	C4D-CHA	2.53	1.47	1.38
30	d	407	LHG	O7-C5	-2.53	1.40	1.46
25	B	609	CLA	C3B-C4B	2.53	1.48	1.42
35	D	403	PHO	C4D-ND	-2.53	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	310	CHL	C1B-C2B	2.53	1.49	1.43
25	5	307	CLA	C1B-C2B	2.53	1.49	1.43
26	q	302	0IE	C17-C16	-2.53	1.40	1.45
24	G	310	CHL	C1B-C2B	2.53	1.49	1.43
24	Y	312	CHL	C1B-NB	-2.53	1.34	1.37
24	r	306	CHL	C4D-CHA	2.53	1.47	1.38
24	G	309	CHL	C1B-C2B	2.53	1.49	1.43
24	y	309	CHL	C1B-NB	-2.53	1.34	1.37
26	y	303	0IE	C6-C7	-2.53	1.40	1.45
25	p	307	CLA	C1B-C2B	2.53	1.49	1.43
24	6	304	CHL	C3B-C4B	2.53	1.48	1.42
24	9	310	CHL	C1B-C2B	2.52	1.49	1.43
24	u	311	CHL	C1B-C2B	2.52	1.49	1.43
24	u	318	CHL	C1B-C2B	2.52	1.49	1.43
24	R	605	CHL	C3B-C4B	2.52	1.48	1.42
24	N	308	CHL	C3B-C4B	2.52	1.48	1.42
25	R	610	CLA	C1B-C2B	2.52	1.49	1.43
25	c	606	CLA	MG-NB	-2.52	2.00	2.05
24	6	309	CHL	C1B-C2B	2.52	1.49	1.43
24	q	310	CHL	C3B-C4B	2.52	1.48	1.42
25	b	609	CLA	C3B-C4B	2.52	1.48	1.42
24	8	315	CHL	C1B-C2B	2.52	1.49	1.43
25	S	610	CLA	C1B-C2B	2.52	1.49	1.43
25	g	317	CLA	C1B-C2B	2.52	1.49	1.43
24	p	312	CHL	MG-NA	-2.52	2.00	2.06
24	3	317	CHL	C1B-C2B	2.52	1.49	1.43
24	G	311	CHL	C1B-C2B	2.52	1.49	1.43
24	1	309	CHL	C4D-CHA	2.52	1.47	1.38
24	2	310	CHL	C4D-CHA	2.52	1.47	1.38
24	1	312	CHL	C4D-CHA	2.52	1.47	1.38
24	s	408	CHL	C3B-C4B	2.52	1.48	1.42
24	2	311	CHL	C4D-CHA	2.52	1.47	1.38
24	6	311	CHL	C4D-CHA	2.52	1.47	1.38
25	N	307	CLA	C1B-C2B	2.52	1.49	1.43
26	2	302	0IE	C6-C7	-2.52	1.40	1.45
25	5	308	CLA	C1B-C2B	2.52	1.49	1.43
24	4	312	CHL	C4D-CHA	2.52	1.47	1.38
35	d	403	PHO	C4D-ND	-2.52	1.35	1.38
24	g	318	CHL	C3B-C4B	2.52	1.48	1.42
24	g	311	CHL	C1B-C2B	2.52	1.49	1.43
24	N	311	CHL	C4D-CHA	2.52	1.47	1.38
24	2	318	CHL	C3B-C4B	2.52	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	311	CHL	C1C-NC	-2.52	1.34	1.37
24	3	304	CHL	C3B-C4B	2.52	1.48	1.42
24	6	310	CHL	C1B-C2B	2.52	1.49	1.43
25	S	612	CLA	C1B-C2B	2.52	1.49	1.43
25	G	317	CLA	C1B-C2B	2.51	1.49	1.43
24	2	311	CHL	C3B-C4B	2.51	1.48	1.42
24	5	318	CHL	C3B-C4B	2.51	1.48	1.42
25	C	601	CLA	MG-NB	-2.51	2.00	2.05
25	y	316	CLA	C3B-C4B	2.51	1.48	1.42
25	2	308	CLA	C1B-C2B	2.51	1.49	1.43
26	Y	302	0IE	C17-C16	-2.51	1.40	1.45
24	3	308	CHL	C1B-C2B	2.51	1.49	1.43
24	8	309	CHL	C3B-C4B	2.51	1.48	1.42
25	c	601	CLA	CMD-C2D	-2.51	1.45	1.50
25	s	411	CLA	C1B-C2B	2.51	1.49	1.43
24	p	312	CHL	C3B-C4B	2.51	1.48	1.42
24	5	311	CHL	C4D-CHA	2.51	1.47	1.38
25	a	605	CLA	C3B-C4B	2.51	1.48	1.42
24	1	310	CHL	C4D-CHA	2.51	1.47	1.38
25	c	601	CLA	C3B-C4B	2.51	1.48	1.42
30	y	319	LHG	O8-C6	-2.51	1.39	1.45
25	A	605	CLA	C3B-C4B	2.51	1.48	1.42
24	4	310	CHL	C4D-CHA	2.51	1.47	1.38
25	2	307	CLA	C1B-C2B	2.51	1.49	1.43
25	s	405	CLA	C3B-C4B	2.51	1.48	1.42
24	y	310	CHL	C1B-NB	-2.51	1.34	1.37
24	Y	308	CHL	C1B-NB	-2.51	1.34	1.37
24	9	317	CHL	C1B-C2B	2.51	1.49	1.43
24	n	311	CHL	C4D-CHA	2.51	1.47	1.38
31	C	614	8CT	C30-C29	2.51	1.54	1.50
25	q	305	CLA	C3B-C4B	2.51	1.48	1.42
35	D	403	PHO	CAC-C3C	-2.51	1.47	1.51
25	C	601	CLA	CMD-C2D	-2.51	1.45	1.50
24	p	311	CHL	C4D-CHA	2.51	1.47	1.38
24	q	309	CHL	C3B-C4B	2.51	1.48	1.42
25	r	305	CLA	C1B-C2B	2.50	1.49	1.43
24	5	311	CHL	C3B-C4B	2.50	1.48	1.42
25	A	607	CLA	C3B-C4B	2.50	1.48	1.42
30	A	601	LHG	O8-C6	-2.50	1.39	1.45
24	3	312	CHL	C1B-C2B	2.50	1.49	1.43
25	Y	315	CLA	MG-NB	-2.50	2.00	2.05
24	G	313	CHL	C4C-C3C	2.50	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	310	CLA	C1B-C2B	2.50	1.49	1.43
30	c	617	LHG	O8-C6	-2.50	1.39	1.45
25	y	316	CLA	MG-NB	-2.50	2.00	2.05
31	c	614	8CT	C30-C29	2.50	1.54	1.50
24	n	309	CHL	MG-NA	-2.50	2.00	2.06
25	c	608	CLA	MG-NB	-2.50	2.00	2.05
26	Y	303	0IE	C6-C7	-2.50	1.40	1.45
24	Y	319	CHL	C3B-C4B	2.50	1.48	1.42
24	3	310	CHL	C1B-C2B	2.50	1.49	1.43
25	Y	314	CLA	C1B-C2B	2.50	1.49	1.43
24	q	307	CHL	C3B-C4B	2.50	1.48	1.42
25	a	603	CLA	C4B-NB	2.50	1.40	1.37
24	1	305	CHL	C4D-CHA	2.50	1.47	1.38
24	7	312	CHL	C3B-C4B	2.50	1.48	1.42
26	5	302	0IE	C13-C12	-2.50	1.40	1.45
24	n	305	CHL	C4D-CHA	2.50	1.47	1.38
24	1	304	CHL	C1B-C2B	2.50	1.49	1.43
25	C	602	CLA	C3B-C4B	2.50	1.48	1.42
24	g	313	CHL	C1B-C2B	2.50	1.49	1.43
24	5	310	CHL	C3B-C4B	2.49	1.48	1.42
24	N	317	CHL	C1B-C2B	2.49	1.49	1.43
25	R	604	CLA	C1B-C2B	2.49	1.49	1.43
26	Y	303	0IE	C17-C16	-2.49	1.40	1.45
24	2	312	CHL	C4D-CHA	2.49	1.47	1.38
24	s	406	CHL	C4D-CHA	2.49	1.47	1.38
25	2	315	CLA	C1B-C2B	2.49	1.49	1.43
24	2	310	CHL	C3B-C4B	2.49	1.48	1.42
24	9	312	CHL	C1B-C2B	2.49	1.49	1.43
25	r	311	CLA	C1B-C2B	2.49	1.49	1.43
24	Y	308	CHL	C3B-C4B	2.49	1.48	1.42
24	6	308	CHL	C1B-C2B	2.49	1.49	1.43
25	y	307	CLA	C1B-C2B	2.49	1.49	1.43
25	a	607	CLA	C4B-NB	2.49	1.40	1.37
24	y	305	CHL	C1C-NC	-2.49	1.34	1.37
30	a	601	LHG	O7-C5	-2.49	1.40	1.46
25	C	606	CLA	CMB-C2B	-2.49	1.45	1.50
30	A	601	LHG	O7-C5	-2.49	1.40	1.46
25	a	605	CLA	MG-NB	-2.49	2.00	2.05
24	u	313	CHL	C1B-C2B	2.49	1.49	1.43
25	7	315	CLA	C1B-C2B	2.49	1.49	1.43
24	8	303	CHL	C3B-C4B	2.49	1.48	1.42
25	C	601	CLA	C3B-C4B	2.49	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	C1B-C2B	2.49	1.49	1.43
24	3	312	CHL	C4C-C3C	2.49	1.49	1.45
24	u	306	CHL	C4D-CHA	2.49	1.47	1.38
24	n	308	CHL	C1B-C2B	2.49	1.49	1.43
25	2	314	CLA	C1B-C2B	2.49	1.49	1.43
24	q	303	CHL	C3B-C4B	2.49	1.48	1.42
24	2	313	CHL	C4D-CHA	2.49	1.47	1.38
24	s	408	CHL	C4D-CHA	2.49	1.47	1.38
24	G	313	CHL	C1B-C2B	2.49	1.49	1.43
26	2	302	0IE	C13-C12	-2.49	1.40	1.45
24	N	305	CHL	C3B-C4B	2.49	1.48	1.42
24	2	312	CHL	C3B-C4B	2.49	1.48	1.42
25	c	605	CLA	MG-NB	-2.49	2.00	2.05
25	c	607	CLA	MG-NB	-2.49	2.00	2.05
26	y	303	0IE	C17-C16	-2.49	1.40	1.45
24	8	310	CHL	C1C-NC	-2.49	1.34	1.37
24	Y	309	CHL	C1B-NB	-2.48	1.34	1.37
25	B	606	CLA	MG-NB	-2.48	2.00	2.05
24	4	308	CHL	C1B-C2B	2.48	1.49	1.43
24	S	613	CHL	C3B-C4B	2.48	1.48	1.42
24	S	605	CHL	C4D-CHA	2.48	1.47	1.38
24	4	305	CHL	C4D-CHA	2.48	1.47	1.38
24	Y	304	CHL	C3B-C4B	2.48	1.48	1.42
24	6	317	CHL	C1B-C2B	2.48	1.49	1.43
25	C	603	CLA	MG-NB	-2.48	2.00	2.05
24	3	305	CHL	C4D-CHA	2.48	1.47	1.38
24	5	312	CHL	C4D-CHA	2.48	1.47	1.38
24	1	308	CHL	C1B-C2B	2.48	1.49	1.43
24	9	309	CHL	C1B-C2B	2.48	1.49	1.43
25	b	604	CLA	C1B-C2B	2.48	1.49	1.43
25	A	607	CLA	MG-NB	-2.48	2.00	2.05
24	p	313	CHL	C1B-NB	-2.48	1.34	1.37
24	5	313	CHL	C1B-C2B	2.48	1.49	1.43
25	5	314	CLA	C1B-C2B	2.48	1.49	1.43
24	u	318	CHL	C4C-C3C	2.48	1.49	1.45
25	a	607	CLA	MG-NB	-2.48	2.00	2.05
26	8	302	0IE	C6-C7	-2.48	1.40	1.45
25	B	610	CLA	MG-NB	-2.48	2.00	2.05
25	A	603	CLA	MG-NB	-2.48	2.00	2.05
24	3	309	CHL	C1B-C2B	2.48	1.49	1.43
25	s	412	CLA	C1B-C2B	2.48	1.49	1.43
24	y	305	CHL	C3B-C4B	2.48	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	309	CHL	C3B-C4B	2.48	1.48	1.42
24	6	305	CHL	C4D-CHA	2.48	1.47	1.38
25	b	606	CLA	MG-NB	-2.48	2.00	2.05
24	S	607	CHL	C4D-CHA	2.48	1.47	1.38
30	C	617	LHG	O8-C6	-2.48	1.39	1.45
25	D	404	CLA	CMD-C2D	-2.48	1.45	1.50
25	5	315	CLA	C1B-C2B	2.48	1.49	1.43
24	N	305	CHL	C4D-CHA	2.47	1.47	1.38
24	5	313	CHL	C4D-CHA	2.47	1.47	1.38
25	C	605	CLA	MG-NB	-2.47	2.00	2.05
25	S	611	CLA	C1B-C2B	2.47	1.49	1.43
26	7	302	0IE	C13-C12	-2.47	1.40	1.45
25	A	603	CLA	C4B-NB	2.47	1.40	1.37
25	Y	306	CLA	C1B-C2B	2.47	1.49	1.43
24	S	606	CHL	C4D-CHA	2.47	1.47	1.38
25	7	314	CLA	C1B-C2B	2.47	1.49	1.43
24	2	309	CHL	C1B-C2B	2.47	1.49	1.43
25	C	601	CLA	C4B-NB	2.47	1.40	1.37
24	s	402	CHL	C3B-C4B	2.47	1.48	1.42
25	p	314	CLA	C1B-C2B	2.47	1.49	1.43
24	N	308	CHL	C1B-C2B	2.47	1.49	1.43
24	9	308	CHL	C4C-C3C	2.47	1.49	1.45
25	C	612	CLA	C1B-C2B	2.47	1.49	1.43
24	S	607	CHL	C3B-C4B	2.47	1.48	1.42
25	c	607	CLA	C3B-C4B	2.47	1.48	1.42
24	g	309	CHL	C4C-C3C	2.47	1.49	1.45
24	9	305	CHL	C4D-CHA	2.47	1.47	1.38
25	b	610	CLA	MG-NB	-2.46	2.00	2.05
24	R	607	CHL	C3B-C4B	2.46	1.48	1.42
25	b	601	CLA	C1B-C2B	2.46	1.49	1.43
24	R	608	CHL	C1B-NB	-2.46	1.34	1.37
25	c	603	CLA	MG-NB	-2.46	2.00	2.05
25	c	610	CLA	MG-NB	-2.46	2.00	2.05
25	B	601	CLA	C1B-C2B	2.46	1.49	1.43
24	5	312	CHL	C3B-C4B	2.46	1.48	1.42
25	B	604	CLA	C1B-C2B	2.46	1.49	1.43
24	7	311	CHL	C4D-CHA	2.46	1.47	1.38
25	c	616	CLA	C3B-C4B	2.46	1.48	1.42
24	p	310	CHL	C4D-CHA	2.46	1.47	1.38
26	r	315	0IE	C13-C12	-2.46	1.40	1.45
25	d	405	CLA	MG-NB	-2.46	2.00	2.05
25	C	616	CLA	C3B-C4B	2.46	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	602	CLA	C3B-C4B	2.46	1.48	1.42
24	4	311	CHL	C4D-CHA	2.46	1.47	1.38
25	B	602	CLA	C1B-C2B	2.46	1.49	1.43
25	C	602	CLA	MG-NB	-2.46	2.00	2.05
24	8	307	CHL	C3B-C4B	2.46	1.48	1.42
25	d	404	CLA	CMD-C2D	-2.46	1.45	1.50
24	Y	305	CHL	C3B-C4B	2.46	1.48	1.42
25	C	607	CLA	C3B-C4B	2.46	1.48	1.42
24	y	306	CHL	C3B-C4B	2.46	1.48	1.42
24	3	311	CHL	C1B-C2B	2.46	1.49	1.43
24	Y	311	CHL	C3B-C4B	2.46	1.48	1.42
25	p	315	CLA	C1B-C2B	2.46	1.49	1.43
24	s	403	CHL	C3B-C4B	2.46	1.48	1.42
24	Y	319	CHL	C1B-NB	-2.45	1.34	1.37
24	6	304	CHL	C1B-C2B	2.45	1.49	1.43
24	6	310	CHL	C4C-C3C	2.45	1.49	1.45
24	r	302	CHL	C1B-C2B	2.45	1.49	1.43
24	7	310	CHL	C4D-CHA	2.45	1.47	1.38
24	r	307	CHL	C1B-NB	-2.45	1.34	1.37
30	a	601	LHG	O8-C6	-2.45	1.39	1.45
30	7	319	LHG	O8-C6	-2.45	1.39	1.45
25	C	607	CLA	MG-NB	-2.45	2.00	2.05
24	1	311	CHL	C4D-CHA	2.45	1.47	1.38
24	5	309	CHL	C1B-C2B	2.45	1.49	1.43
24	8	307	CHL	C1B-NB	-2.45	1.34	1.37
26	R	614	0IE	C13-C12	-2.45	1.40	1.45
25	y	315	CLA	C3B-C4B	2.45	1.48	1.42
30	G	319	LHG	O8-C6	-2.45	1.39	1.45
24	u	310	CHL	C1B-C2B	2.45	1.49	1.43
25	c	611	CLA	C1B-C2B	2.45	1.49	1.43
24	s	403	CHL	C1C-NC	-2.45	1.34	1.37
24	n	317	CHL	C4C-C3C	2.45	1.49	1.45
24	N	309	CHL	C1B-C2B	2.45	1.49	1.43
25	y	316	CLA	C1B-C2B	2.45	1.49	1.43
26	5	302	0IE	C17-C16	-2.45	1.40	1.45
24	S	602	CHL	C1C-NC	-2.45	1.34	1.37
24	r	308	CHL	C4D-CHA	2.45	1.47	1.38
24	s	407	CHL	C4D-CHA	2.45	1.47	1.38
24	7	313	CHL	C1B-NB	-2.45	1.34	1.37
24	3	304	CHL	C1B-C2B	2.44	1.49	1.43
24	N	312	CHL	C3B-C4B	2.44	1.48	1.42
24	n	309	CHL	C1B-C2B	2.44	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	318	CHL	C1B-C2B	2.44	1.49	1.43
25	B	606	CLA	C1B-C2B	2.44	1.49	1.43
24	s	409	CHL	C3B-C4B	2.44	1.48	1.42
24	S	601	CHL	C3B-C4B	2.44	1.48	1.42
26	p	303	0IE	C6-C7	-2.44	1.40	1.45
24	S	602	CHL	C3B-C4B	2.44	1.48	1.42
30	A	612	LHG	O8-C6	-2.44	1.39	1.45
24	R	606	CHL	C4D-CHA	2.44	1.47	1.38
25	c	609	CLA	MG-NB	-2.44	2.00	2.05
24	R	607	CHL	C1B-C2B	2.44	1.49	1.43
24	r	307	CHL	C4D-CHA	2.44	1.47	1.38
30	y	319	LHG	O7-C5	-2.44	1.40	1.46
24	7	309	CHL	C4C-C3C	2.44	1.49	1.45
24	s	406	CHL	C1B-NB	-2.44	1.34	1.37
25	Y	314	CLA	C3B-C4B	2.44	1.48	1.42
25	c	604	CLA	C1B-C2B	2.44	1.49	1.43
24	n	309	CHL	C3B-C4B	2.44	1.48	1.42
26	2	302	0IE	C17-C16	-2.44	1.40	1.45
25	a	604	CLA	CMB-C2B	-2.44	1.45	1.50
26	q	302	0IE	C6-C7	-2.44	1.40	1.45
25	B	615	CLA	C1B-C2B	2.44	1.49	1.43
25	y	315	CLA	C1B-C2B	2.44	1.49	1.43
24	q	309	CHL	C4D-CHA	2.44	1.47	1.38
25	Y	315	CLA	C3B-C4B	2.44	1.48	1.42
24	y	311	CHL	C3B-C4B	2.44	1.48	1.42
24	p	305	CHL	C1B-C2B	2.44	1.49	1.43
24	g	313	CHL	C4C-C3C	2.43	1.49	1.45
30	p	319	LHG	O8-C6	-2.43	1.39	1.45
25	C	608	CLA	MG-NB	-2.43	2.01	2.05
25	c	602	CLA	MG-NB	-2.43	2.01	2.05
24	2	311	CHL	C1B-C2B	2.43	1.49	1.43
24	N	312	CHL	C1B-C2B	2.43	1.49	1.43
24	s	409	CHL	C4D-CHA	2.43	1.47	1.38
24	p	318	CHL	C1B-C2B	2.43	1.49	1.43
24	6	312	CHL	C4C-C3C	2.43	1.49	1.45
24	u	305	CHL	C4C-C3C	2.43	1.49	1.45
24	5	306	CHL	C3B-C4B	2.43	1.48	1.42
24	n	312	CHL	C3B-C4B	2.43	1.48	1.42
24	y	312	CHL	C3B-C4B	2.43	1.48	1.42
24	n	304	CHL	C1B-C2B	2.43	1.49	1.43
24	R	607	CHL	C4D-CHA	2.43	1.47	1.38
25	A	604	CLA	MG-NB	-2.43	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C3B-C4B	2.43	1.48	1.42
24	S	608	CHL	C1B-C2B	2.43	1.49	1.43
24	5	318	CHL	C1B-C2B	2.43	1.49	1.43
24	r	308	CHL	C1B-C2B	2.43	1.49	1.43
25	B	603	CLA	C3B-C4B	2.43	1.48	1.42
24	9	312	CHL	C4C-C3C	2.43	1.49	1.45
25	D	405	CLA	MG-NB	-2.43	2.01	2.05
24	3	310	CHL	C4C-C3C	2.43	1.49	1.45
26	p	302	0IE	C13-C12	-2.43	1.40	1.45
24	N	309	CHL	C3B-C4B	2.43	1.48	1.42
24	4	312	CHL	C1B-C2B	2.43	1.49	1.43
24	r	308	CHL	C3B-C4B	2.43	1.48	1.42
26	7	303	0IE	C6-C7	-2.43	1.40	1.45
25	q	305	CLA	MG-NB	-2.42	2.01	2.05
24	6	305	CHL	C3B-C4B	2.42	1.48	1.42
24	5	311	CHL	C1B-C2B	2.42	1.49	1.43
30	g	319	LHG	O8-C6	-2.42	1.39	1.45
24	3	305	CHL	C3B-C4B	2.42	1.48	1.42
24	R	601	CHL	C1B-C2B	2.42	1.49	1.43
24	2	305	CHL	C1B-C2B	2.42	1.49	1.43
25	B	605	CLA	C1B-C2B	2.42	1.49	1.43
25	S	603	CLA	MG-NB	-2.42	2.01	2.05
25	b	606	CLA	C1B-C2B	2.42	1.49	1.43
24	7	312	CHL	C4D-CHA	2.42	1.47	1.38
25	y	316	CLA	CMC-C2C	-2.42	1.45	1.50
25	c	612	CLA	C1B-C2B	2.42	1.49	1.43
24	Y	310	CHL	C4D-CHA	2.42	1.47	1.38
26	p	302	0IE	C17-C16	-2.42	1.40	1.45
24	R	608	CHL	C4D-CHA	2.42	1.47	1.38
24	r	309	CHL	C4D-CHA	2.42	1.47	1.38
24	1	310	CHL	C1B-C2B	2.42	1.49	1.43
24	s	409	CHL	C1B-C2B	2.42	1.49	1.43
24	y	313	CHL	C1C-NC	-2.42	1.34	1.37
25	D	405	CLA	C1B-C2B	2.42	1.49	1.43
25	q	306	CLA	C1B-C2B	2.42	1.49	1.43
24	2	318	CHL	C1B-NB	-2.42	1.34	1.37
24	3	308	CHL	C4C-C3C	2.42	1.49	1.45
25	S	611	CLA	MG-NB	-2.42	2.01	2.05
24	2	306	CHL	C3B-C4B	2.42	1.48	1.42
25	C	609	CLA	MG-NB	-2.42	2.01	2.05
25	s	413	CLA	MG-NB	-2.42	2.01	2.05
24	n	312	CHL	C4D-CHA	2.42	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	613	CHL	C4D-CHA	2.42	1.47	1.38
23	f	201	HEM	FE-NA	2.42	2.03	1.95
25	b	613	CLA	MG-NB	-2.42	2.01	2.05
24	q	303	CHL	C1B-NB	-2.42	1.34	1.37
24	R	606	CHL	C1B-C2B	2.42	1.48	1.43
24	N	312	CHL	C4D-CHA	2.42	1.47	1.38
25	C	610	CLA	MG-NB	-2.42	2.01	2.05
24	S	608	CHL	C3B-C4B	2.42	1.48	1.42
24	7	305	CHL	C1B-C2B	2.42	1.48	1.43
25	b	616	CLA	CMC-C2C	-2.42	1.45	1.50
24	S	608	CHL	C4D-CHA	2.42	1.47	1.38
24	Y	319	CHL	C4D-CHA	2.42	1.47	1.38
24	u	313	CHL	C4C-C3C	2.42	1.49	1.45
25	a	603	CLA	MG-NB	-2.42	2.01	2.05
25	8	306	CLA	C1B-C2B	2.42	1.48	1.43
31	c	615	8CT	C33-C32	-2.42	1.43	1.50
24	p	313	CHL	C3B-C4B	2.42	1.48	1.42
24	1	309	CHL	C1B-C2B	2.42	1.48	1.43
25	b	609	CLA	C1B-C2B	2.42	1.48	1.43
24	6	308	CHL	C4C-C3C	2.42	1.49	1.45
30	a	612	LHG	O8-C6	-2.42	1.39	1.45
24	8	303	CHL	C1B-NB	-2.41	1.34	1.37
24	5	305	CHL	C1B-C2B	2.41	1.48	1.43
24	p	309	CHL	C4C-C3C	2.41	1.49	1.45
30	Y	318	LHG	O7-C5	-2.41	1.40	1.46
24	Y	311	CHL	C4D-CHA	2.41	1.47	1.38
24	y	312	CHL	C4D-CHA	2.41	1.47	1.38
25	d	405	CLA	C1B-C2B	2.41	1.48	1.43
24	n	312	CHL	C1B-C2B	2.41	1.48	1.43
25	Y	315	CLA	C1B-C2B	2.41	1.48	1.43
25	b	602	CLA	C1B-C2B	2.41	1.48	1.43
24	Y	310	CHL	C1B-NB	-2.41	1.34	1.37
25	y	317	CLA	MG-NB	-2.41	2.01	2.05
24	s	414	CHL	C3B-C4B	2.41	1.48	1.42
24	S	613	CHL	C1B-NB	-2.41	1.34	1.37
25	B	611	CLA	MG-NB	-2.41	2.01	2.05
24	Y	317	CHL	C1B-NB	-2.41	1.34	1.37
25	b	608	CLA	MG-NB	-2.41	2.01	2.05
24	G	306	CHL	C4D-CHA	2.41	1.47	1.38
24	4	312	CHL	C3B-C4B	2.41	1.48	1.42
24	r	303	CHL	C4D-CHA	2.41	1.47	1.38
25	Y	315	CLA	CMC-C2C	-2.41	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	MG-NB	-2.41	2.01	2.05
25	B	609	CLA	C1B-C2B	2.41	1.48	1.43
26	g	303	0IE	C6-C7	-2.41	1.40	1.45
25	b	607	CLA	C1B-C2B	2.41	1.48	1.43
24	N	310	CHL	C1B-C2B	2.41	1.48	1.43
24	n	310	CHL	C1B-C2B	2.41	1.48	1.43
25	b	605	CLA	C1B-C2B	2.41	1.48	1.43
24	p	313	CHL	C4D-CHA	2.41	1.47	1.38
25	C	601	CLA	C1B-C2B	2.41	1.48	1.43
24	r	309	CHL	C1B-NB	-2.41	1.34	1.37
25	B	604	CLA	MG-NB	-2.41	2.01	2.05
24	7	318	CHL	C1B-C2B	2.41	1.48	1.43
25	a	604	CLA	MG-NB	-2.41	2.01	2.05
24	R	606	CHL	C1B-NB	-2.41	1.34	1.37
24	1	305	CHL	C1B-C2B	2.41	1.48	1.43
30	4	318	LHG	O8-C6	-2.41	1.39	1.45
25	b	602	CLA	MG-NB	-2.41	2.01	2.05
24	y	311	CHL	C4D-CHA	2.41	1.47	1.38
24	p	312	CHL	C4D-CHA	2.40	1.46	1.38
26	6	302	0IE	C13-C12	-2.40	1.40	1.45
24	S	605	CHL	C3B-C4B	2.40	1.48	1.42
24	8	303	CHL	C1B-C2B	2.40	1.48	1.43
24	1	312	CHL	C3B-C4B	2.40	1.48	1.42
24	Y	312	CHL	C1C-NC	-2.40	1.34	1.37
24	1	312	CHL	C1B-NB	-2.40	1.34	1.37
24	Y	317	CHL	C4D-CHA	2.40	1.46	1.38
24	q	311	CHL	C3B-C4B	2.40	1.48	1.42
24	4	309	CHL	C1B-C2B	2.40	1.48	1.43
25	b	615	CLA	MG-NB	-2.40	2.01	2.05
26	7	302	0IE	C17-C16	-2.40	1.40	1.45
24	N	304	CHL	C1B-C2B	2.40	1.48	1.43
24	2	313	CHL	C1B-C2B	2.40	1.48	1.43
25	B	607	CLA	C1B-C2B	2.40	1.48	1.43
24	Y	305	CHL	C1C-NC	-2.40	1.34	1.37
25	s	412	CLA	MG-NB	-2.40	2.01	2.05
24	Y	310	CHL	C3B-C4B	2.40	1.48	1.42
24	7	312	CHL	C1B-C2B	2.40	1.48	1.43
30	a	612	LHG	O7-C5	-2.40	1.40	1.46
25	B	613	CLA	MG-NB	-2.40	2.01	2.05
24	N	317	CHL	C4C-C3C	2.40	1.49	1.45
25	A	604	CLA	CMB-C2B	-2.40	1.45	1.50
24	s	414	CHL	C4D-CHA	2.40	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	607	CLA	C1B-C2B	2.40	1.48	1.43
25	C	604	CLA	C1B-C2B	2.40	1.48	1.43
24	r	309	CHL	C3B-C4B	2.40	1.48	1.42
24	r	307	CHL	C1B-C2B	2.40	1.48	1.43
26	3	302	0IE	C6-C7	-2.40	1.40	1.45
24	u	309	CHL	C4C-C3C	2.40	1.49	1.45
24	s	406	CHL	C3B-C4B	2.40	1.48	1.42
24	S	601	CHL	C4D-CHA	2.40	1.46	1.38
25	C	611	CLA	C1B-C2B	2.40	1.48	1.43
30	A	612	LHG	O7-C5	-2.39	1.40	1.46
25	C	604	CLA	MG-NB	-2.39	2.01	2.05
31	C	615	8CT	C33-C32	-2.39	1.43	1.50
26	3	302	0IE	C13-C12	-2.39	1.40	1.45
24	8	310	CHL	C3B-C4B	2.39	1.48	1.42
25	b	616	CLA	C3B-C4B	2.39	1.48	1.42
25	S	612	CLA	MG-NB	-2.39	2.01	2.05
25	Y	313	CLA	MG-NB	-2.39	2.01	2.05
24	s	402	CHL	C1C-NC	-2.39	1.34	1.37
24	y	318	CHL	C4D-CHA	2.39	1.46	1.38
24	r	309	CHL	C1B-C2B	2.39	1.48	1.43
25	C	616	CLA	C1B-C2B	2.39	1.48	1.43
25	y	314	CLA	MG-NB	-2.39	2.01	2.05
25	b	611	CLA	MG-NB	-2.39	2.01	2.05
25	d	404	CLA	MG-NB	-2.39	2.01	2.05
24	q	310	CHL	C4D-CHA	2.39	1.46	1.38
24	R	608	CHL	C1B-C2B	2.39	1.48	1.43
25	B	616	CLA	CMC-C2C	-2.39	1.45	1.50
25	c	607	CLA	C1B-C2B	2.39	1.48	1.43
24	4	317	CHL	C4C-C3C	2.39	1.49	1.45
24	1	312	CHL	C1B-C2B	2.39	1.48	1.43
25	d	404	CLA	C1B-C2B	2.39	1.48	1.43
24	R	602	CHL	C4D-CHA	2.39	1.46	1.38
24	S	601	CHL	C1B-NB	-2.39	1.34	1.37
24	N	309	CHL	C4D-CHA	2.39	1.46	1.38
25	b	603	CLA	CMD-C2D	-2.39	1.45	1.50
25	Y	306	CLA	MG-NB	-2.39	2.01	2.05
26	6	302	0IE	C6-C7	-2.39	1.40	1.45
25	B	616	CLA	MG-NB	-2.39	2.01	2.05
26	G	303	0IE	C6-C7	-2.38	1.40	1.45
25	c	601	CLA	C1B-C2B	2.38	1.48	1.43
24	y	306	CHL	C1C-NC	-2.38	1.34	1.37
24	4	310	CHL	C1B-C2B	2.38	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	307	CLA	C1B-C2B	2.38	1.48	1.43
25	b	616	CLA	MG-NB	-2.38	2.01	2.05
25	8	305	CLA	MG-NB	-2.38	2.01	2.05
25	y	307	CLA	MG-NB	-2.38	2.01	2.05
24	q	316	CHL	C4C-C3C	2.38	1.49	1.45
24	s	402	CHL	C4D-CHA	2.38	1.46	1.38
25	y	308	CLA	C1B-C2B	2.38	1.48	1.43
24	5	312	CHL	C1B-C2B	2.38	1.48	1.43
25	B	614	CLA	MG-NB	-2.38	2.01	2.05
24	Y	308	CHL	C1B-C2B	2.38	1.48	1.43
24	Y	317	CHL	C1C-NC	-2.38	1.34	1.37
24	5	306	CHL	C1C-NC	-2.38	1.34	1.37
24	7	313	CHL	C4D-CHA	2.38	1.46	1.38
25	b	604	CLA	MG-NB	-2.38	2.01	2.05
24	y	318	CHL	C1B-NB	-2.38	1.34	1.37
25	B	616	CLA	C3B-C4B	2.38	1.48	1.42
24	1	311	CHL	C1B-NB	-2.38	1.34	1.37
25	B	603	CLA	C1B-C2B	2.38	1.48	1.43
24	G	310	CHL	C4C-C3C	2.38	1.49	1.45
24	8	309	CHL	C4D-CHA	2.38	1.46	1.38
24	s	402	CHL	C1B-NB	-2.38	1.34	1.37
24	1	304	CHL	C4C-C3C	2.38	1.49	1.45
24	1	317	CHL	C4C-C3C	2.38	1.49	1.45
24	g	306	CHL	C1B-C2B	2.38	1.48	1.43
24	S	605	CHL	C1B-NB	-2.38	1.34	1.37
24	g	306	CHL	C4D-CHA	2.38	1.46	1.38
30	1	318	LHG	O8-C6	-2.38	1.39	1.45
30	n	318	LHG	O8-C6	-2.38	1.39	1.45
25	c	602	CLA	CMC-C2C	-2.38	1.45	1.50
24	y	309	CHL	C1B-C2B	2.38	1.48	1.43
25	D	404	CLA	C1B-C2B	2.38	1.48	1.43
24	R	602	CHL	C3B-C4B	2.38	1.48	1.42
24	5	318	CHL	C1B-NB	-2.37	1.34	1.37
24	r	303	CHL	C3B-C4B	2.37	1.48	1.42
24	7	313	CHL	C3B-C4B	2.37	1.48	1.42
26	G	303	0IE	C17-C16	-2.37	1.40	1.45
24	R	605	CHL	C1B-C2B	2.37	1.48	1.43
24	2	312	CHL	C1B-C2B	2.37	1.48	1.43
24	q	304	CHL	C4D-CHA	2.37	1.46	1.38
24	q	311	CHL	C4D-CHA	2.37	1.46	1.38
25	Y	316	CLA	MG-NB	-2.37	2.01	2.05
24	S	605	CHL	C1B-C2B	2.37	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	311	CLA	C1B-C2B	2.37	1.48	1.43
30	D	408	LHG	O7-C5	-2.37	1.40	1.46
24	6	311	CHL	C1B-C2B	2.37	1.48	1.43
25	B	605	CLA	MG-NB	-2.37	2.01	2.05
24	p	312	CHL	C1B-C2B	2.37	1.48	1.43
24	r	306	CHL	C1B-C2B	2.37	1.48	1.43
25	b	614	CLA	MG-NB	-2.37	2.01	2.05
24	p	311	CHL	C1B-NB	-2.37	1.34	1.37
24	8	304	CHL	C4D-CHA	2.37	1.46	1.38
24	q	303	CHL	C1B-C2B	2.37	1.48	1.43
26	2	303	0IE	C17-C16	-2.37	1.40	1.45
25	Y	314	CLA	MG-NB	-2.37	2.01	2.05
24	Y	311	CHL	C1C-NC	-2.37	1.34	1.37
25	B	615	CLA	MG-NB	-2.37	2.01	2.05
24	s	403	CHL	C1B-NB	-2.37	1.34	1.37
26	N	302	0IE	C13-C12	-2.37	1.40	1.45
25	b	609	CLA	MG-NB	-2.37	2.01	2.05
24	Y	312	CHL	C3B-C4B	2.37	1.48	1.42
24	S	607	CHL	C1B-C2B	2.37	1.48	1.43
24	r	303	CHL	C1B-C2B	2.37	1.48	1.43
25	c	616	CLA	C1B-C2B	2.37	1.48	1.43
24	2	306	CHL	C4D-CHA	2.37	1.46	1.38
25	B	604	CLA	C3B-C4B	2.37	1.48	1.42
24	G	305	CHL	C1B-C2B	2.37	1.48	1.43
26	g	303	0IE	C17-C16	-2.37	1.40	1.45
25	a	603	CLA	CMD-C2D	-2.37	1.45	1.50
26	5	303	0IE	C17-C16	-2.37	1.40	1.45
24	2	306	CHL	C1C-NC	-2.37	1.34	1.37
25	B	603	CLA	CMD-C2D	-2.37	1.45	1.50
24	y	311	CHL	C1B-NB	-2.37	1.34	1.37
24	s	408	CHL	C1B-C2B	2.37	1.48	1.43
25	8	311	CLA	MG-NB	-2.36	2.01	2.05
24	G	309	CHL	C4C-C3C	2.36	1.49	1.45
24	S	606	CHL	C1B-C2B	2.36	1.48	1.43
25	8	313	CLA	MG-NB	-2.36	2.01	2.05
25	y	315	CLA	MG-NB	-2.36	2.01	2.05
25	c	612	CLA	MG-NB	-2.36	2.01	2.05
24	p	311	CHL	C1B-C2B	2.36	1.48	1.43
25	7	307	CLA	MG-NB	-2.36	2.01	2.05
23	E	201	HEM	FE-NC	2.36	2.03	1.95
24	y	313	CHL	C4D-CHA	2.36	1.46	1.38
24	R	602	CHL	C1B-C2B	2.36	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	310	CHL	C4D-CHA	2.36	1.46	1.38
24	R	601	CHL	C4C-C3C	2.36	1.49	1.45
24	s	409	CHL	C4C-C3C	2.36	1.49	1.45
25	s	404	CLA	MG-NB	-2.36	2.01	2.05
26	p	303	0IE	C13-C12	-2.36	1.40	1.45
25	S	610	CLA	MG-NB	-2.36	2.01	2.05
25	p	316	CLA	MG-NB	-2.36	2.01	2.05
24	Y	311	CHL	C1B-NB	-2.36	1.34	1.37
24	q	307	CHL	C1B-NB	-2.36	1.34	1.37
24	7	306	CHL	C1B-NB	-2.36	1.34	1.37
24	G	306	CHL	C1B-C2B	2.36	1.48	1.43
24	R	608	CHL	C3B-C4B	2.36	1.48	1.42
35	A	606	PHO	C3B-C2B	-2.36	1.37	1.40
24	p	305	CHL	C4D-CHA	2.36	1.46	1.38
25	q	314	CLA	MG-NB	-2.36	2.01	2.05
24	S	606	CHL	C1B-NB	-2.36	1.34	1.37
24	7	311	CHL	C1B-C2B	2.36	1.48	1.43
26	4	302	0IE	C13-C12	-2.36	1.40	1.45
24	2	306	CHL	C1B-NB	-2.36	1.34	1.37
25	s	411	CLA	MG-NB	-2.36	2.01	2.05
31	s	415	8CT	C25-C26	2.36	1.38	1.35
24	R	605	CHL	C4D-CHA	2.36	1.46	1.38
25	C	602	CLA	CMB-C2B	-2.36	1.45	1.50
24	y	309	CHL	C1C-NC	-2.35	1.34	1.37
24	6	305	CHL	C1B-C2B	2.35	1.48	1.43
25	c	603	CLA	C1B-C2B	2.35	1.48	1.43
24	y	306	CHL	C4D-CHA	2.35	1.46	1.38
24	p	313	CHL	C1B-C2B	2.35	1.48	1.43
24	5	306	CHL	C4D-CHA	2.35	1.46	1.38
24	s	403	CHL	C4D-CHA	2.35	1.46	1.38
24	Y	305	CHL	C4D-CHA	2.35	1.46	1.38
24	q	309	CHL	C1B-C2B	2.35	1.48	1.43
25	B	614	CLA	C1B-C2B	2.35	1.48	1.43
24	q	310	CHL	C1C-NC	-2.35	1.34	1.37
24	y	313	CHL	C3B-C4B	2.35	1.48	1.42
25	B	612	CLA	CMB-C2B	-2.35	1.45	1.50
25	8	306	CLA	MG-NB	-2.35	2.01	2.05
25	b	603	CLA	C1B-C2B	2.35	1.48	1.43
25	b	614	CLA	C1B-C2B	2.35	1.48	1.43
24	5	313	CHL	C1B-NB	-2.35	1.34	1.37
25	B	608	CLA	MG-NB	-2.35	2.01	2.05
24	q	309	CHL	C1C-NC	-2.35	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	614	8CT	C30-C29	2.35	1.53	1.50
24	u	310	CHL	C4C-C3C	2.35	1.49	1.45
25	C	616	CLA	CMD-C2D	-2.35	1.45	1.50
30	N	318	LHG	O8-C6	-2.35	1.39	1.45
24	4	305	CHL	C1B-C2B	2.35	1.48	1.43
24	g	305	CHL	C1B-C2B	2.35	1.48	1.43
26	g	302	0IE	C17-C16	-2.35	1.40	1.45
24	y	305	CHL	C4D-CHA	2.35	1.46	1.38
24	s	403	CHL	C1B-C2B	2.35	1.48	1.43
24	N	304	CHL	C4C-C3C	2.35	1.49	1.45
25	C	602	CLA	C1B-C2B	2.35	1.48	1.43
25	p	307	CLA	MG-NB	-2.35	2.01	2.05
24	s	406	CHL	C1B-C2B	2.35	1.48	1.43
24	s	407	CHL	C1B-C2B	2.35	1.48	1.43
24	R	608	CHL	C1C-NC	-2.35	1.34	1.37
24	n	309	CHL	C4D-CHA	2.35	1.46	1.38
26	R	614	0IE	C17-C16	-2.34	1.40	1.45
24	q	316	CHL	C1B-NB	-2.34	1.34	1.37
24	4	311	CHL	C1B-C2B	2.34	1.48	1.43
24	7	305	CHL	C4D-CHA	2.34	1.46	1.38
25	B	609	CLA	MG-NB	-2.34	2.01	2.05
24	1	311	CHL	C1B-C2B	2.34	1.48	1.43
24	Y	319	CHL	C1B-C2B	2.34	1.48	1.43
30	4	318	LHG	O8-C23	2.34	1.40	1.33
24	9	309	CHL	C4C-C3C	2.34	1.49	1.45
25	4	313	CLA	CHC-C1C	2.34	1.43	1.38
25	b	604	CLA	C3B-C4B	2.34	1.48	1.42
25	C	602	CLA	CMC-C2C	-2.34	1.45	1.50
24	9	304	CHL	C4C-C3C	2.34	1.49	1.45
23	E	201	HEM	FE-NA	2.34	2.03	1.95
24	4	311	CHL	C1B-NB	-2.34	1.34	1.37
24	7	311	CHL	C1B-NB	-2.34	1.34	1.37
24	9	305	CHL	C1B-C2B	2.34	1.48	1.43
24	Y	308	CHL	C1C-NC	-2.34	1.34	1.37
25	C	612	CLA	MG-NB	-2.34	2.01	2.05
26	5	303	0IE	C13-C12	-2.34	1.40	1.45
24	S	602	CHL	C4D-CHA	2.34	1.46	1.38
25	c	602	CLA	CMB-C2B	-2.34	1.45	1.50
24	9	312	CHL	C1B-NB	-2.34	1.34	1.37
25	q	312	CLA	C1B-C2B	2.34	1.48	1.43
25	y	314	CLA	CMB-C2B	-2.34	1.45	1.50
24	2	313	CHL	C1B-NB	-2.34	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	304	CHL	C4D-CHA	2.34	1.46	1.38
24	g	310	CHL	C4C-C3C	2.34	1.49	1.45
24	S	602	CHL	C1B-C2B	2.33	1.48	1.43
25	C	603	CLA	C1B-C2B	2.33	1.48	1.43
24	7	318	CHL	C1B-NB	-2.33	1.34	1.37
25	A	603	CLA	CMD-C2D	-2.33	1.45	1.50
25	c	610	CLA	CMD-C2D	-2.33	1.45	1.50
24	G	318	CHL	C1B-NB	-2.33	1.34	1.37
24	4	304	CHL	C4C-C3C	2.33	1.49	1.45
24	3	305	CHL	C1B-C2B	2.33	1.48	1.43
26	7	303	0IE	C13-C12	-2.33	1.40	1.45
25	y	308	CLA	MG-NB	-2.33	2.01	2.05
25	b	601	CLA	MG-NB	-2.33	2.01	2.05
26	g	302	0IE	C13-C12	-2.33	1.40	1.45
26	g	303	0IE	C13-C12	-2.33	1.40	1.45
24	1	310	CHL	C1B-NB	-2.33	1.34	1.37
24	8	315	CHL	C1B-NB	-2.33	1.34	1.37
24	N	312	CHL	C4C-C3C	2.33	1.49	1.45
24	7	312	CHL	C1C-NC	-2.33	1.34	1.37
25	c	604	CLA	MG-NB	-2.33	2.01	2.05
25	r	305	CLA	MG-NB	-2.33	2.01	2.05
25	7	316	CLA	MG-NB	-2.33	2.01	2.05
24	n	317	CHL	C1B-NB	-2.33	1.34	1.37
30	1	318	LHG	O8-C23	2.33	1.40	1.33
24	Y	312	CHL	C4D-CHA	2.33	1.46	1.38
25	C	611	CLA	MG-NB	-2.33	2.01	2.05
25	b	612	CLA	CMB-C2B	-2.33	1.45	1.50
25	c	611	CLA	MG-NB	-2.33	2.01	2.05
25	C	610	CLA	CMD-C2D	-2.33	1.45	1.50
24	G	305	CHL	C1B-NB	-2.33	1.34	1.37
24	N	317	CHL	C1B-NB	-2.33	1.34	1.37
24	s	414	CHL	C1B-NB	-2.33	1.34	1.37
24	1	309	CHL	C4C-C3C	2.33	1.49	1.45
25	D	404	CLA	MG-NB	-2.33	2.01	2.05
24	q	304	CHL	C1C-NC	-2.33	1.34	1.37
30	p	319	LHG	O7-C5	-2.33	1.40	1.46
24	1	304	CHL	C1B-NB	-2.33	1.34	1.37
24	4	312	CHL	C1B-NB	-2.33	1.34	1.37
26	9	302	0IE	C13-C12	-2.33	1.40	1.45
24	y	318	CHL	C1C-NC	-2.33	1.34	1.37
24	8	309	CHL	C1C-NC	-2.33	1.34	1.37
24	s	408	CHL	C1C-NC	-2.33	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	309	CHL	C4C-C3C	2.33	1.49	1.45
26	G	303	0IE	C13-C12	-2.33	1.40	1.45
26	5	303	0IE	C6-C7	-2.32	1.41	1.45
24	8	315	CHL	C4C-C3C	2.32	1.49	1.45
26	2	303	0IE	C13-C12	-2.32	1.41	1.45
26	u	302	0IE	C13-C12	-2.32	1.41	1.45
24	n	304	CHL	C4C-C3C	2.32	1.49	1.45
25	b	604	CLA	CMB-C2B	-2.32	1.45	1.50
24	n	311	CHL	C1B-C2B	2.32	1.48	1.43
25	q	312	CLA	MG-NB	-2.32	2.01	2.05
24	g	318	CHL	C1B-NB	-2.32	1.34	1.37
24	p	306	CHL	C1B-NB	-2.32	1.34	1.37
24	Y	309	CHL	C4D-CHA	2.32	1.46	1.38
25	c	616	CLA	CMD-C2D	-2.32	1.45	1.50
25	Y	307	CLA	MG-NB	-2.32	2.01	2.05
24	Y	319	CHL	C1C-NC	-2.32	1.34	1.37
24	1	311	CHL	C4C-C3C	2.32	1.49	1.45
24	4	309	CHL	C4C-C3C	2.32	1.49	1.45
26	G	302	0IE	C6-C7	-2.32	1.41	1.45
24	r	307	CHL	C1C-NC	-2.32	1.34	1.37
24	y	310	CHL	C4D-CHA	2.32	1.46	1.38
39	d	406	PL9	C31-C29	-2.32	1.46	1.51
25	r	305	CLA	CMB-C2B	-2.32	1.45	1.50
31	s	416	8CT	C33-C32	-2.32	1.44	1.50
24	2	313	CHL	C1C-NC	-2.32	1.34	1.37
24	n	312	CHL	C4C-C3C	2.32	1.49	1.45
25	b	603	CLA	CMB-C2B	-2.32	1.45	1.50
24	n	310	CHL	C1B-NB	-2.32	1.34	1.37
25	C	609	CLA	CMB-C2B	-2.32	1.45	1.50
31	C	613	8CT	C33-C32	-2.32	1.44	1.50
30	7	319	LHG	O7-C7	2.32	1.40	1.34
26	1	302	0IE	C13-C12	-2.32	1.41	1.45
25	2	307	CLA	MG-NB	-2.32	2.01	2.05
25	5	315	CLA	MG-NB	-2.32	2.01	2.05
24	3	312	CHL	C1B-NB	-2.32	1.34	1.37
25	y	314	CLA	C1B-C2B	2.32	1.48	1.43
24	y	312	CHL	C1C-NC	-2.31	1.34	1.37
25	A	603	CLA	CMC-C2C	-2.31	1.45	1.50
24	9	310	CHL	C4C-C3C	2.31	1.49	1.45
24	s	407	CHL	C1B-NB	-2.31	1.34	1.37
24	3	309	CHL	C4C-C3C	2.31	1.49	1.45
30	9	318	LHG	O8-C6	-2.31	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	601	CHL	C1C-NC	-2.31	1.34	1.37
24	8	309	CHL	C1B-C2B	2.31	1.48	1.43
26	r	315	0IE	C17-C16	-2.31	1.41	1.45
30	9	318	LHG	O8-C23	2.31	1.40	1.33
24	p	310	CHL	C1B-C2B	2.31	1.48	1.43
25	B	608	CLA	C1B-C2B	2.31	1.48	1.43
24	N	305	CHL	C1B-C2B	2.31	1.48	1.43
25	y	317	CLA	C1B-C2B	2.31	1.48	1.43
24	7	306	CHL	C4D-CHA	2.31	1.46	1.38
24	u	306	CHL	C1B-C2B	2.31	1.48	1.43
25	Y	315	CLA	CMD-C2D	-2.31	1.45	1.50
26	2	303	0IE	C6-C7	-2.31	1.41	1.45
24	9	317	CHL	C1B-NB	-2.31	1.34	1.37
25	1	313	CLA	CHC-C1C	2.31	1.43	1.38
25	B	601	CLA	MG-NB	-2.31	2.01	2.05
25	q	306	CLA	MG-NB	-2.31	2.01	2.05
25	B	603	CLA	CMB-C2B	-2.31	1.45	1.50
24	p	305	CHL	C3B-C4B	2.31	1.48	1.42
24	u	311	CHL	C4C-C3C	2.31	1.49	1.45
24	G	318	CHL	C1B-C2B	2.31	1.48	1.43
24	g	318	CHL	C1B-C2B	2.31	1.48	1.43
24	S	608	CHL	C1C-NC	-2.31	1.34	1.37
24	8	308	CHL	C4D-CHA	2.31	1.46	1.38
24	G	309	CHL	C1B-NB	-2.31	1.34	1.37
24	8	308	CHL	C1C-NC	-2.31	1.34	1.37
24	u	311	CHL	C1B-NB	-2.31	1.34	1.37
25	b	607	CLA	MG-NB	-2.31	2.01	2.05
25	B	611	CLA	CMC-C2C	-2.30	1.45	1.50
26	G	302	0IE	C17-C16	-2.30	1.41	1.45
26	4	302	0IE	C17-C16	-2.30	1.41	1.45
24	r	309	CHL	C1C-NC	-2.30	1.34	1.37
25	s	405	CLA	MG-NB	-2.30	2.01	2.05
24	S	602	CHL	C1B-NB	-2.30	1.35	1.37
26	p	303	0IE	C17-C16	-2.30	1.41	1.45
25	u	317	CLA	CHC-C1C	2.30	1.43	1.38
24	p	313	CHL	C1C-NC	-2.30	1.34	1.37
24	s	409	CHL	C1C-NC	-2.30	1.34	1.37
24	Y	310	CHL	C1B-C2B	2.30	1.48	1.43
25	y	316	CLA	CMD-C2D	-2.30	1.45	1.50
25	9	316	CLA	CHC-C1C	2.30	1.43	1.38
30	n	318	LHG	O8-C23	2.30	1.40	1.33
25	c	607	CLA	CMD-C2D	-2.30	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	414	CHL	C1C-NC	-2.30	1.34	1.37
26	n	302	0IE	C13-C12	-2.30	1.41	1.45
24	y	311	CHL	C1B-C2B	2.30	1.48	1.43
24	q	307	CHL	C1B-C2B	2.30	1.48	1.43
25	S	604	CLA	MG-NB	-2.30	2.01	2.05
24	q	308	CHL	C4D-CHA	2.30	1.46	1.38
24	g	305	CHL	C1B-NB	-2.30	1.35	1.37
26	g	302	0IE	C6-C7	-2.30	1.41	1.45
26	n	302	0IE	C6-C7	-2.30	1.41	1.45
24	G	312	CHL	C4C-C3C	2.30	1.49	1.45
25	r	312	CLA	MG-NB	-2.30	2.01	2.05
24	1	312	CHL	C4C-C3C	2.30	1.49	1.45
24	8	304	CHL	C1C-NC	-2.30	1.34	1.37
25	b	605	CLA	MG-NB	-2.30	2.01	2.05
26	N	302	0IE	C6-C7	-2.30	1.41	1.45
24	n	305	CHL	C1B-C2B	2.30	1.48	1.43
24	5	305	CHL	C1C-NC	-2.30	1.34	1.37
26	1	302	0IE	C6-C7	-2.30	1.41	1.45
24	4	310	CHL	C1B-NB	-2.30	1.35	1.37
31	S	614	8CT	C25-C26	2.30	1.38	1.35
25	r	311	CLA	MG-NB	-2.30	2.01	2.05
24	R	602	CHL	C1B-NB	-2.30	1.35	1.37
24	G	313	CHL	C1B-NB	-2.30	1.35	1.37
25	C	607	CLA	CMD-C2D	-2.30	1.45	1.50
30	N	318	LHG	O8-C23	2.30	1.40	1.33
24	7	313	CHL	C1B-C2B	2.30	1.48	1.43
24	p	306	CHL	C4D-CHA	2.30	1.46	1.38
25	Y	313	CLA	CMB-C2B	-2.30	1.45	1.50
24	Y	317	CHL	C1B-C2B	2.29	1.48	1.43
25	Y	313	CLA	C1B-C2B	2.29	1.48	1.43
25	c	602	CLA	C1B-C2B	2.29	1.48	1.43
24	N	308	CHL	C1C-NC	-2.29	1.34	1.37
25	c	609	CLA	CMB-C2B	-2.29	1.45	1.50
24	Y	317	CHL	C3B-C4B	2.29	1.48	1.42
30	N	318	LHG	O7-C7	2.29	1.40	1.34
26	7	303	0IE	C17-C16	-2.29	1.41	1.45
24	3	305	CHL	C1B-NB	-2.29	1.35	1.37
24	7	306	CHL	CHB-C4A	-2.29	1.32	1.37
24	N	311	CHL	C1B-C2B	2.29	1.48	1.43
24	N	310	CHL	C1B-NB	-2.29	1.35	1.37
25	5	307	CLA	MG-NB	-2.29	2.01	2.05
25	a	603	CLA	CMC-C2C	-2.29	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	CMC-C2C	-2.29	1.45	1.50
25	b	608	CLA	C1B-C2B	2.29	1.48	1.43
31	S	615	8CT	C33-C32	-2.29	1.44	1.50
24	S	608	CHL	C4C-C3C	2.29	1.49	1.45
24	6	310	CHL	C1B-NB	-2.29	1.35	1.37
25	7	314	CLA	MG-NB	-2.29	2.01	2.05
25	Y	316	CLA	C1B-C2B	2.29	1.48	1.43
24	g	312	CHL	C4C-C3C	2.29	1.49	1.45
25	B	607	CLA	MG-NB	-2.29	2.01	2.05
24	Y	305	CHL	CHB-C4A	-2.29	1.32	1.37
26	1	302	0IE	C17-C16	-2.29	1.41	1.45
31	x	601	8CT	C33-C32	-2.29	1.44	1.50
24	8	303	CHL	C1C-NC	-2.29	1.34	1.37
25	R	604	CLA	MG-NB	-2.29	2.01	2.05
24	1	308	CHL	C4C-C3C	2.29	1.49	1.45
24	q	310	CHL	C1B-C2B	2.29	1.48	1.43
24	y	306	CHL	CHB-C4A	-2.29	1.32	1.37
30	p	319	LHG	O7-C7	2.28	1.40	1.34
24	g	311	CHL	C4C-C3C	2.28	1.49	1.45
26	3	302	0IE	C17-C16	-2.28	1.41	1.45
25	b	609	CLA	CMB-C2B	-2.28	1.46	1.50
24	p	306	CHL	C1C-NC	-2.28	1.34	1.37
25	a	607	CLA	C1B-C2B	2.28	1.48	1.43
24	s	407	CHL	C1C-NC	-2.28	1.34	1.37
26	3	303	0IE	C6-C7	-2.28	1.41	1.45
24	5	310	CHL	C1B-C2B	2.28	1.48	1.43
31	a	608	8CT	C33-C32	-2.28	1.44	1.50
24	8	307	CHL	C1C-NC	-2.28	1.34	1.37
25	b	603	CLA	CMC-C2C	-2.28	1.46	1.50
30	5	319	LHG	O8-C23	2.28	1.40	1.33
25	s	417	CLA	MG-NB	-2.28	2.01	2.05
25	a	604	CLA	CMD-C2D	-2.28	1.46	1.50
24	q	307	CHL	C1C-NC	-2.28	1.34	1.37
24	7	310	CHL	C1B-C2B	2.28	1.48	1.43
24	4	309	CHL	C1B-NB	-2.28	1.35	1.37
24	y	312	CHL	C1B-NB	-2.28	1.35	1.37
25	2	315	CLA	MG-NB	-2.28	2.01	2.05
31	s	415	8CT	C30-C29	2.28	1.53	1.50
24	S	613	CHL	C1C-NC	-2.28	1.34	1.37
24	g	313	CHL	C1B-NB	-2.28	1.35	1.37
25	b	606	CLA	CMD-C2D	-2.28	1.46	1.50
24	Y	310	CHL	C1C-NC	-2.28	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	304	CHL	C1B-NB	-2.28	1.35	1.37
25	Y	314	CLA	CMD-C2D	-2.28	1.46	1.50
25	2	317	CLA	MG-NB	-2.28	2.01	2.05
24	4	312	CHL	C4C-C3C	2.28	1.49	1.45
24	R	601	CHL	C1C-NC	-2.28	1.34	1.37
39	D	406	PL9	C36-C34	-2.28	1.46	1.51
24	y	318	CHL	C1B-C2B	2.28	1.48	1.43
24	R	602	CHL	C1C-NC	-2.28	1.34	1.37
24	u	313	CHL	C1B-NB	-2.28	1.35	1.37
26	7	302	0IE	C6-C7	-2.27	1.41	1.45
24	q	308	CHL	C1C-NC	-2.27	1.34	1.37
31	A	608	8CT	C33-C32	-2.27	1.44	1.50
26	3	303	0IE	C17-C16	-2.27	1.41	1.45
25	B	603	CLA	CMC-C2C	-2.27	1.46	1.50
25	c	608	CLA	CMC-C2C	-2.27	1.46	1.50
31	X	601	8CT	C33-C32	-2.27	1.44	1.50
30	n	318	LHG	O7-C7	2.27	1.40	1.34
25	C	608	CLA	CMC-C2C	-2.27	1.46	1.50
24	r	302	CHL	C4C-C3C	2.27	1.49	1.45
24	S	606	CHL	C1C-NC	-2.27	1.34	1.37
24	S	607	CHL	C1C-NC	-2.27	1.34	1.37
25	c	609	CLA	CMC-C2C	-2.27	1.46	1.50
24	2	310	CHL	C1B-C2B	2.27	1.48	1.43
24	4	308	CHL	C4C-C3C	2.27	1.49	1.45
26	G	302	0IE	C13-C12	-2.27	1.41	1.45
26	9	303	0IE	C17-C16	-2.27	1.41	1.45
24	n	308	CHL	C1B-NB	-2.27	1.35	1.37
25	s	412	CLA	CMD-C2D	-2.27	1.46	1.50
24	y	305	CHL	C1B-C2B	2.27	1.48	1.43
26	4	302	0IE	C6-C7	-2.27	1.41	1.45
26	6	302	0IE	C17-C16	-2.27	1.41	1.45
25	A	605	CLA	C1B-C2B	2.27	1.48	1.43
25	u	314	CLA	CHC-C1C	2.27	1.43	1.38
24	g	311	CHL	C1B-NB	-2.27	1.35	1.37
24	3	309	CHL	C1C-NC	-2.27	1.34	1.37
24	5	306	CHL	C1B-C2B	2.27	1.48	1.43
25	A	607	CLA	C1B-C2B	2.27	1.48	1.43
30	G	319	LHG	O8-C23	2.27	1.40	1.33
24	9	305	CHL	C4C-C3C	2.27	1.48	1.45
24	u	318	CHL	C1B-NB	-2.27	1.35	1.37
24	4	311	CHL	C4C-C3C	2.27	1.48	1.45
26	u	302	0IE	C6-C7	-2.27	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	306	CHL	C1B-NB	-2.27	1.35	1.37
25	c	610	CLA	C1B-C2B	2.27	1.48	1.43
24	6	312	CHL	C1B-NB	-2.27	1.35	1.37
24	6	304	CHL	C4C-C3C	2.27	1.48	1.45
31	c	613	8CT	C33-C32	-2.27	1.44	1.50
24	S	601	CHL	C1B-C2B	2.26	1.48	1.43
25	R	604	CLA	CMB-C2B	-2.26	1.46	1.50
24	5	311	CHL	C4C-C3C	2.26	1.48	1.45
30	7	319	LHG	O7-C5	-2.26	1.40	1.46
24	2	309	CHL	C1B-NB	-2.26	1.35	1.37
24	g	309	CHL	C1B-NB	-2.26	1.35	1.37
25	R	611	CLA	MG-NB	-2.26	2.01	2.05
25	B	604	CLA	CMD-C2D	-2.26	1.46	1.50
30	9	318	LHG	O7-C7	2.26	1.40	1.34
24	1	309	CHL	C1B-NB	-2.26	1.35	1.37
24	7	309	CHL	C1B-NB	-2.26	1.35	1.37
24	2	311	CHL	C4C-C3C	2.26	1.48	1.45
25	p	314	CLA	MG-NB	-2.26	2.01	2.05
32	B	618	SQD	O2-C2	-2.26	1.37	1.43
24	3	310	CHL	C1B-NB	-2.26	1.35	1.37
25	B	605	CLA	CMD-C2D	-2.26	1.46	1.50
24	5	305	CHL	C4C-C3C	2.26	1.48	1.45
25	C	608	CLA	CMD-C2D	-2.26	1.46	1.50
26	p	302	0IE	C6-C7	-2.26	1.41	1.45
24	S	608	CHL	C1B-NB	-2.26	1.35	1.37
24	s	409	CHL	C1B-NB	-2.26	1.35	1.37
25	3	313	CLA	CHC-C1C	2.26	1.43	1.38
24	p	306	CHL	CHB-C4A	-2.26	1.32	1.37
24	9	310	CHL	C1B-NB	-2.26	1.35	1.37
26	R	614	0IE	C6-C7	-2.26	1.41	1.45
24	q	303	CHL	C1C-NC	-2.26	1.34	1.37
25	8	312	CLA	MG-NB	-2.26	2.01	2.05
24	7	305	CHL	C3B-C4B	2.26	1.48	1.42
24	S	601	CHL	CHB-C4A	-2.26	1.32	1.37
24	y	311	CHL	C1C-NC	-2.26	1.34	1.37
24	G	318	CHL	C4C-C3C	2.26	1.48	1.45
25	5	314	CLA	MG-NB	-2.26	2.01	2.05
25	B	608	CLA	CMB-C2B	-2.26	1.46	1.50
24	n	304	CHL	C1B-NB	-2.26	1.35	1.37
24	7	306	CHL	C1C-NC	-2.26	1.34	1.37
24	5	309	CHL	C4C-C3C	2.26	1.48	1.45
25	B	604	CLA	CMB-C2B	-2.26	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	308	CLA	MG-NB	-2.26	2.01	2.05
24	6	317	CHL	C4C-C3C	2.26	1.48	1.45
24	1	305	CHL	C1B-NB	-2.26	1.35	1.37
30	2	319	LHG	O8-C23	2.26	1.39	1.33
25	A	605	CLA	CMB-C2B	-2.25	1.46	1.50
30	5	319	LHG	O8-C6	-2.25	1.40	1.45
24	y	310	CHL	CHB-C4A	-2.25	1.32	1.37
24	r	306	CHL	C1B-NB	-2.25	1.35	1.37
24	p	309	CHL	C1B-NB	-2.25	1.35	1.37
25	a	605	CLA	C1B-C2B	2.25	1.48	1.43
30	c	617	LHG	O7-C7	2.25	1.40	1.34
30	N	318	LHG	O7-C5	-2.25	1.41	1.46
25	B	613	CLA	C1B-C2B	2.25	1.48	1.43
25	B	613	CLA	CMB-C2B	-2.25	1.46	1.50
26	r	315	0IE	C6-C7	-2.25	1.41	1.45
24	1	311	CHL	C1C-NC	-2.25	1.34	1.37
24	Y	309	CHL	CHB-C4A	-2.25	1.32	1.37
25	C	610	CLA	C1B-C2B	2.25	1.48	1.43
25	y	315	CLA	CMD-C2D	-2.25	1.46	1.50
25	7	315	CLA	MG-NB	-2.25	2.01	2.05
24	y	310	CHL	C1C-NC	-2.25	1.34	1.37
25	b	608	CLA	CMB-C2B	-2.25	1.46	1.50
24	4	305	CHL	C1B-NB	-2.25	1.35	1.37
30	5	319	LHG	O7-C5	-2.25	1.41	1.46
30	G	319	LHG	O7-C7	2.25	1.40	1.34
25	B	609	CLA	CMB-C2B	-2.25	1.46	1.50
24	1	312	CHL	C1C-NC	-2.25	1.34	1.37
25	S	616	CLA	MG-NB	-2.25	2.01	2.05
25	8	311	CLA	CMB-C2B	-2.25	1.46	1.50
25	S	609	CLA	MG-NB	-2.25	2.01	2.05
24	p	311	CHL	C1C-NC	-2.25	1.34	1.37
24	q	311	CHL	CHB-C4A	-2.25	1.32	1.37
24	8	307	CHL	C1B-C2B	2.25	1.48	1.43
24	s	402	CHL	CHB-C4A	-2.25	1.32	1.37
24	p	318	CHL	C1B-NB	-2.25	1.35	1.37
25	b	614	CLA	CMD-C2D	-2.25	1.46	1.50
29	5	301	0UR	C19-C18	2.25	1.53	1.50
24	G	311	CHL	C1B-NB	-2.25	1.35	1.37
24	r	303	CHL	C1C-NC	-2.25	1.34	1.37
24	7	313	CHL	C1C-NC	-2.25	1.34	1.37
30	n	318	LHG	O7-C5	-2.25	1.41	1.46
30	a	612	LHG	O8-C23	2.25	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	CMD-C2D	-2.25	1.46	1.50
25	c	605	CLA	C1B-C2B	2.25	1.48	1.43
25	C	609	CLA	CMC-C2C	-2.25	1.46	1.50
25	b	607	CLA	CMB-C2B	-2.25	1.46	1.50
24	R	606	CHL	C1C-NC	-2.25	1.34	1.37
25	D	404	CLA	CMB-C2B	-2.25	1.46	1.50
24	2	310	CHL	C1B-NB	-2.25	1.35	1.37
24	r	308	CHL	C1B-NB	-2.25	1.35	1.37
24	7	311	CHL	C1C-NC	-2.25	1.34	1.37
24	s	402	CHL	C1B-C2B	2.24	1.48	1.43
24	6	305	CHL	C1B-NB	-2.24	1.35	1.37
24	3	311	CHL	C4C-C3C	2.24	1.48	1.45
25	9	313	CLA	CHC-C1C	2.24	1.43	1.38
25	R	610	CLA	MG-NB	-2.24	2.01	2.05
29	2	301	0UR	C19-C18	2.24	1.53	1.50
26	3	303	0IE	C13-C12	-2.24	1.41	1.45
24	5	318	CHL	C4C-C3C	2.24	1.48	1.45
24	Y	304	CHL	C1B-C2B	2.24	1.48	1.43
24	R	601	CHL	C1B-NB	-2.24	1.35	1.37
25	b	604	CLA	CMD-C2D	-2.24	1.46	1.50
25	d	405	CLA	CMD-C2D	-2.24	1.46	1.50
30	p	319	LHG	O8-C23	2.24	1.39	1.33
24	5	313	CHL	C1C-NC	-2.24	1.34	1.37
30	2	319	LHG	O7-C5	-2.24	1.41	1.46
31	C	614	8CT	C33-C32	-2.24	1.44	1.50
24	u	306	CHL	C1B-NB	-2.24	1.35	1.37
35	a	606	PHO	C3B-C2B	-2.24	1.37	1.40
25	A	610	CLA	CHC-C1C	2.24	1.43	1.38
30	g	319	LHG	O8-C23	2.24	1.39	1.33
30	A	612	LHG	O8-C23	2.24	1.39	1.33
24	6	304	CHL	C1C-NC	-2.24	1.34	1.37
25	R	603	CLA	MG-NB	-2.24	2.01	2.05
25	b	613	CLA	CMD-C2D	-2.24	1.46	1.50
25	q	313	CLA	MG-NB	-2.24	2.01	2.05
25	6	313	CLA	CHC-C1C	2.24	1.43	1.38
24	5	310	CHL	C1B-NB	-2.24	1.35	1.37
25	q	312	CLA	CMB-C2B	-2.24	1.46	1.50
30	C	617	LHG	O7-C7	2.24	1.40	1.34
24	5	318	CHL	C1C-NC	-2.24	1.34	1.37
24	y	318	CHL	C3B-C4B	2.24	1.48	1.42
24	r	303	CHL	C1B-NB	-2.24	1.35	1.37
25	u	315	CLA	CHC-C1C	2.24	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	304	CLA	MG-NB	-2.24	2.01	2.05
31	s	415	8CT	C33-C32	-2.24	1.44	1.50
24	q	304	CHL	CHB-C4A	-2.24	1.32	1.37
25	a	605	CLA	CMB-C2B	-2.24	1.46	1.50
30	7	319	LHG	O8-C23	2.24	1.39	1.33
24	r	302	CHL	C1C-NC	-2.24	1.34	1.37
25	N	307	CLA	CHC-C1C	2.24	1.43	1.38
24	g	318	CHL	C4C-C3C	2.24	1.48	1.45
24	5	309	CHL	C1B-NB	-2.23	1.35	1.37
24	5	311	CHL	C1C-NC	-2.23	1.34	1.37
30	2	319	LHG	O8-C6	-2.23	1.40	1.45
24	N	310	CHL	C4C-C3C	2.23	1.48	1.45
25	A	603	CLA	C1B-C2B	2.23	1.48	1.43
25	d	404	CLA	CMB-C2B	-2.23	1.46	1.50
30	4	318	LHG	O7-C7	2.23	1.40	1.34
39	D	406	PL9	C31-C29	-2.23	1.46	1.51
25	p	315	CLA	MG-NB	-2.23	2.01	2.05
24	2	318	CHL	C1C-NC	-2.23	1.34	1.37
25	Y	313	CLA	CMD-C2D	-2.23	1.46	1.50
25	c	610	CLA	CMC-C2C	-2.23	1.46	1.50
25	s	410	CLA	MG-NB	-2.23	2.01	2.05
25	Y	315	CLA	CMB-C2B	-2.23	1.46	1.50
25	2	314	CLA	MG-NB	-2.23	2.01	2.05
24	2	306	CHL	C1B-C2B	2.23	1.48	1.43
24	9	308	CHL	C1B-NB	-2.23	1.35	1.37
24	r	302	CHL	C1B-NB	-2.23	1.35	1.37
24	Y	309	CHL	C1C-NC	-2.23	1.34	1.37
25	g	317	CLA	MG-NB	-2.23	2.01	2.05
25	S	611	CLA	CMD-C2D	-2.23	1.46	1.50
25	Y	316	CLA	CMD-C2D	-2.23	1.46	1.50
24	3	304	CHL	C4C-C3C	2.23	1.48	1.45
24	5	311	CHL	C1B-NB	-2.23	1.35	1.37
24	5	313	CHL	C4C-C3C	2.23	1.48	1.45
24	7	305	CHL	C1B-NB	-2.23	1.35	1.37
25	b	614	CLA	CMB-C2B	-2.23	1.46	1.50
25	C	606	CLA	C1B-C2B	2.23	1.48	1.43
24	n	308	CHL	C4C-C3C	2.23	1.48	1.45
25	4	306	CLA	MG-NB	-2.23	2.01	2.05
24	n	310	CHL	C4C-C3C	2.23	1.48	1.45
26	N	302	0IE	C17-C16	-2.23	1.41	1.45
28	g	304	NEX	O24-C25	-2.23	1.43	1.46
32	b	618	SQD	O2-C2	-2.23	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	302	0IE	C17-C16	-2.23	1.41	1.45
26	9	303	0IE	C13-C12	-2.23	1.41	1.45
24	u	310	CHL	C1C-NC	-2.22	1.34	1.37
25	8	306	CLA	CMB-C2B	-2.22	1.46	1.50
25	5	316	CLA	CMC-C2C	-2.22	1.46	1.50
30	C	617	LHG	O7-C5	-2.22	1.41	1.46
24	p	310	CHL	C1B-NB	-2.22	1.35	1.37
24	2	309	CHL	C1C-NC	-2.22	1.34	1.37
24	2	310	CHL	C1C-NC	-2.22	1.34	1.37
24	5	309	CHL	C1C-NC	-2.22	1.34	1.37
25	b	610	CLA	CMD-C2D	-2.22	1.46	1.50
24	8	304	CHL	CHB-C4A	-2.22	1.32	1.37
24	8	310	CHL	CHB-C4A	-2.22	1.32	1.37
24	3	309	CHL	C1B-NB	-2.22	1.35	1.37
25	D	404	CLA	CMC-C2C	-2.22	1.46	1.50
25	4	316	CLA	CHC-C1C	2.22	1.43	1.38
25	3	306	CLA	MG-NB	-2.22	2.01	2.05
25	5	308	CLA	MG-NB	-2.22	2.01	2.05
24	7	310	CHL	C4C-C3C	2.22	1.48	1.45
25	B	610	CLA	C1B-C2B	2.22	1.48	1.43
25	B	606	CLA	CMD-C2D	-2.22	1.46	1.50
24	9	309	CHL	C1C-NC	-2.22	1.34	1.37
24	6	309	CHL	C1C-NC	-2.22	1.34	1.37
24	n	309	CHL	C1C-NC	-2.22	1.34	1.37
24	p	312	CHL	C1C-NC	-2.22	1.34	1.37
30	1	318	LHG	O7-C5	-2.22	1.41	1.46
25	R	609	CLA	MG-NB	-2.22	2.01	2.05
30	g	319	LHG	O7-C7	2.22	1.40	1.34
25	D	405	CLA	CMD-C2D	-2.22	1.46	1.50
25	C	604	CLA	CMD-C2D	-2.22	1.46	1.50
24	N	309	CHL	C1C-NC	-2.22	1.34	1.37
25	8	314	CLA	MG-NB	-2.22	2.01	2.05
25	b	610	CLA	C1B-C2B	2.22	1.48	1.43
24	2	309	CHL	C4C-C3C	2.22	1.48	1.45
25	y	317	CLA	CMD-C2D	-2.22	1.46	1.50
25	c	609	CLA	CMD-C2D	-2.22	1.46	1.50
24	2	313	CHL	C4C-C3C	2.22	1.48	1.45
24	G	306	CHL	C1B-NB	-2.22	1.35	1.37
25	B	612	CLA	CMD-C2D	-2.22	1.46	1.50
24	N	312	CHL	C1C-NC	-2.22	1.34	1.37
32	D	409	SQD	O2-C2	-2.22	1.37	1.43
25	A	604	CLA	CMD-C2D	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	CMD-C2D	-2.22	1.46	1.50
25	d	404	CLA	CMC-C2C	-2.22	1.46	1.50
25	A	605	CLA	CMD-C2D	-2.22	1.46	1.50
25	b	611	CLA	C1B-C2B	2.22	1.48	1.43
26	u	302	0IE	C17-C16	-2.22	1.41	1.45
25	B	610	CLA	CMB-C2B	-2.22	1.46	1.50
25	1	316	CLA	CHC-C1C	2.22	1.43	1.38
25	b	612	CLA	CMD-C2D	-2.22	1.46	1.50
31	S	614	8CT	C33-C32	-2.22	1.44	1.50
25	C	616	CLA	CMB-C2B	-2.22	1.46	1.50
25	5	317	CLA	MG-NB	-2.22	2.01	2.05
25	G	317	CLA	CHC-C1C	2.22	1.43	1.38
24	N	311	CHL	C1B-NB	-2.22	1.35	1.37
24	g	312	CHL	C1B-NB	-2.22	1.35	1.37
25	c	606	CLA	C1B-C2B	2.22	1.48	1.43
25	n	313	CLA	CHC-C1C	2.21	1.43	1.38
25	q	305	CLA	CMB-C2B	-2.21	1.46	1.50
24	p	318	CHL	C1C-NC	-2.21	1.34	1.37
24	7	310	CHL	C1C-NC	-2.21	1.34	1.37
24	u	309	CHL	C1B-NB	-2.21	1.35	1.37
24	n	311	CHL	C1B-NB	-2.21	1.35	1.37
25	G	314	CLA	CHC-C1C	2.21	1.43	1.38
24	2	305	CHL	C4C-C3C	2.21	1.48	1.45
25	y	314	CLA	CMD-C2D	-2.21	1.46	1.50
25	c	605	CLA	CMB-C2B	-2.21	1.46	1.50
25	p	308	CLA	MG-NB	-2.21	2.01	2.05
24	6	304	CHL	C1B-NB	-2.21	1.35	1.37
24	3	317	CHL	C4C-C3C	2.21	1.48	1.45
24	4	308	CHL	C1B-NB	-2.21	1.35	1.37
24	g	306	CHL	C4C-C3C	2.21	1.48	1.45
26	u	303	0IE	C17-C16	-2.21	1.41	1.45
24	7	318	CHL	C4C-C3C	2.21	1.48	1.45
24	R	607	CHL	C1C-NC	-2.21	1.34	1.37
25	p	307	CLA	CMD-C2D	-2.21	1.46	1.50
24	s	414	CHL	C1B-C2B	2.21	1.48	1.43
25	B	602	CLA	CMD-C2D	-2.21	1.46	1.50
25	C	610	CLA	CMB-C2B	-2.21	1.46	1.50
25	a	607	CLA	CMB-C2B	-2.21	1.46	1.50
25	c	608	CLA	CMD-C2D	-2.21	1.46	1.50
24	2	311	CHL	C1B-NB	-2.21	1.35	1.37
24	n	312	CHL	C1B-NB	-2.21	1.35	1.37
25	B	606	CLA	CMC-C2C	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	q	315	CLA	MG-NB	-2.21	2.01	2.05
26	n	302	0IE	C17-C16	-2.21	1.41	1.45
24	2	318	CHL	C4C-C3C	2.21	1.48	1.45
25	a	603	CLA	C1B-C2B	2.21	1.48	1.43
25	c	606	CLA	CMD-C2D	-2.21	1.46	1.50
24	y	305	CHL	C1B-NB	-2.21	1.35	1.37
24	1	309	CHL	C1C-NC	-2.21	1.34	1.37
25	g	317	CLA	CHC-C1C	2.21	1.43	1.38
24	Y	311	CHL	C1B-C2B	2.21	1.48	1.43
24	G	306	CHL	C4C-C3C	2.21	1.48	1.45
24	2	305	CHL	C1C-NC	-2.21	1.34	1.37
25	C	605	CLA	CMB-C2B	-2.21	1.46	1.50
25	c	607	CLA	CMB-C2B	-2.21	1.46	1.50
28	1	303	NEX	O24-C25	-2.21	1.43	1.46
30	1	318	LHG	O7-C7	2.21	1.40	1.34
24	s	406	CHL	C1C-NC	-2.21	1.34	1.37
25	4	307	CLA	MG-NB	-2.21	2.01	2.05
25	b	616	CLA	CMB-C2B	-2.21	1.46	1.50
24	9	311	CHL	C1B-NB	-2.21	1.35	1.37
24	7	310	CHL	C1B-NB	-2.21	1.35	1.37
25	B	605	CLA	CMB-C2B	-2.20	1.46	1.50
25	B	610	CLA	CMD-C2D	-2.20	1.46	1.50
32	d	409	SQD	O2-C2	-2.20	1.37	1.43
25	N	313	CLA	CHC-C1C	2.20	1.43	1.38
24	4	317	CHL	C1B-NB	-2.20	1.35	1.37
24	6	309	CHL	C1B-NB	-2.20	1.35	1.37
31	c	614	8CT	C33-C32	-2.20	1.44	1.50
24	G	313	CHL	C1C-NC	-2.20	1.34	1.37
25	C	605	CLA	C1B-C2B	2.20	1.48	1.43
30	g	319	LHG	O7-C5	-2.20	1.41	1.46
26	9	302	0IE	C6-C7	-2.20	1.41	1.45
25	C	602	CLA	CMD-C2D	-2.20	1.46	1.50
25	b	613	CLA	CMB-C2B	-2.20	1.46	1.50
24	8	308	CHL	CHB-C4A	-2.20	1.32	1.37
25	r	310	CLA	CMC-C2C	-2.20	1.46	1.50
26	9	303	0IE	C6-C7	-2.20	1.41	1.45
24	u	306	CHL	C4C-C3C	2.20	1.48	1.45
24	9	312	CHL	C1C-NC	-2.20	1.34	1.37
24	r	308	CHL	C1C-NC	-2.20	1.34	1.37
25	8	305	CLA	CMB-C2B	-2.20	1.46	1.50
25	2	316	CLA	CMC-C2C	-2.20	1.46	1.50
24	y	312	CHL	C1B-C2B	2.20	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	315	CLA	CMB-C2B	-2.20	1.46	1.50
28	p	304	NEX	O24-C25	-2.20	1.43	1.46
25	1	306	CLA	MG-NB	-2.20	2.01	2.05
25	B	615	CLA	CMC-C2C	-2.20	1.46	1.50
24	u	310	CHL	C1B-NB	-2.20	1.35	1.37
25	b	602	CLA	CMD-C2D	-2.20	1.46	1.50
24	4	312	CHL	C1C-NC	-2.20	1.34	1.37
25	D	405	CLA	CMB-C2B	-2.20	1.46	1.50
25	c	603	CLA	CMD-C2D	-2.20	1.46	1.50
25	B	611	CLA	C1B-C2B	2.20	1.48	1.43
25	5	316	CLA	MG-NB	-2.20	2.01	2.05
25	C	607	CLA	CMB-C2B	-2.20	1.46	1.50
25	y	316	CLA	CMB-C2B	-2.20	1.46	1.50
25	b	610	CLA	CMB-C2B	-2.20	1.46	1.50
25	1	314	CLA	CHC-C1C	2.20	1.43	1.38
24	N	308	CHL	C1B-NB	-2.20	1.35	1.37
24	5	305	CHL	C1B-NB	-2.20	1.35	1.37
32	a	609	SQD	O2-C2	-2.20	1.37	1.43
24	q	307	CHL	C4C-C3C	2.20	1.48	1.45
25	b	613	CLA	C1B-C2B	2.20	1.48	1.43
24	u	305	CHL	C1B-NB	-2.19	1.35	1.37
25	c	612	CLA	CMD-C2D	-2.19	1.46	1.50
25	G	316	CLA	MG-NB	-2.19	2.01	2.05
24	Y	312	CHL	CHB-C4A	-2.19	1.32	1.37
25	B	613	CLA	CMD-C2D	-2.19	1.46	1.50
25	g	315	CLA	CHC-C1C	2.19	1.43	1.38
24	1	308	CHL	C1B-NB	-2.19	1.35	1.37
25	G	317	CLA	MG-NB	-2.19	2.01	2.05
25	r	310	CLA	MG-NB	-2.19	2.01	2.05
25	n	307	CLA	CHC-C1C	2.19	1.43	1.38
25	N	306	CLA	MG-NB	-2.19	2.01	2.05
25	s	405	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	606	CLA	CMD-C2D	-2.19	1.46	1.50
25	b	605	CLA	CMB-C2B	-2.19	1.46	1.50
24	N	305	CHL	C1B-NB	-2.19	1.35	1.37
24	G	311	CHL	C4C-C3C	2.19	1.48	1.45
25	g	307	CLA	CHC-C1C	2.19	1.43	1.38
25	a	610	CLA	CHC-C1C	2.19	1.43	1.38
25	B	607	CLA	CMB-C2B	-2.19	1.46	1.50
24	5	312	CHL	C4C-C3C	2.19	1.48	1.45
24	n	312	CHL	C1C-NC	-2.19	1.34	1.37
24	N	308	CHL	C4C-C3C	2.19	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	609	CLA	CMD-C2D	-2.19	1.46	1.50
30	Y	318	LHG	O8-C23	2.19	1.39	1.33
25	S	604	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	612	CLA	CMD-C2D	-2.19	1.46	1.50
30	G	319	LHG	O7-C5	-2.19	1.41	1.46
25	n	314	CLA	CHC-C1C	2.19	1.43	1.38
24	g	318	CHL	C1C-NC	-2.19	1.34	1.37
24	p	310	CHL	C1C-NC	-2.19	1.34	1.37
30	4	318	LHG	O7-C5	-2.19	1.41	1.46
25	1	307	CLA	MG-NB	-2.19	2.01	2.05
24	q	303	CHL	C4C-C3C	2.19	1.48	1.45
25	q	305	CLA	CMD-C2D	-2.19	1.46	1.50
24	Y	308	CHL	C4C-C3C	2.19	1.48	1.45
25	c	611	CLA	CMC-C2C	-2.19	1.46	1.50
24	R	607	CHL	C1B-NB	-2.19	1.35	1.37
24	9	309	CHL	C1B-NB	-2.19	1.35	1.37
24	6	311	CHL	C4C-C3C	2.19	1.48	1.45
24	p	318	CHL	C4C-C3C	2.19	1.48	1.45
25	C	612	CLA	CMB-C2B	-2.19	1.46	1.50
24	N	312	CHL	C1B-NB	-2.18	1.35	1.37
25	y	307	CLA	CMB-C2B	-2.18	1.46	1.50
25	c	602	CLA	CMD-C2D	-2.18	1.46	1.50
24	S	613	CHL	C1B-C2B	2.18	1.48	1.43
24	3	311	CHL	C1C-NC	-2.18	1.34	1.37
24	G	310	CHL	C1C-NC	-2.18	1.34	1.37
24	g	305	CHL	C1C-NC	-2.18	1.34	1.37
25	c	616	CLA	CMB-C2B	-2.18	1.46	1.50
25	g	316	CLA	MG-NB	-2.18	2.01	2.05
24	3	308	CHL	C1B-NB	-2.18	1.35	1.37
25	Y	314	CLA	CMB-C2B	-2.18	1.46	1.50
24	u	305	CHL	C1C-NC	-2.18	1.34	1.37
24	5	312	CHL	C1B-NB	-2.18	1.35	1.37
25	c	611	CLA	CMB-C2B	-2.18	1.46	1.50
30	c	617	LHG	O7-C5	-2.18	1.41	1.46
25	G	315	CLA	CHC-C1C	2.18	1.43	1.38
25	b	609	CLA	CMD-C2D	-2.18	1.46	1.50
25	a	605	CLA	CMD-C2D	-2.18	1.46	1.50
25	r	310	CLA	CMD-C2D	-2.18	1.46	1.50
26	u	303	0IE	C6-C7	-2.18	1.41	1.45
24	g	313	CHL	C1C-NC	-2.18	1.34	1.37
24	1	310	CHL	C4C-C3C	2.18	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	611	CLA	CMD-C2D	-2.18	1.46	1.50
25	c	610	CLA	CMB-C2B	-2.18	1.46	1.50
30	y	319	LHG	O8-C23	2.18	1.39	1.33
24	y	309	CHL	C4C-C3C	2.18	1.48	1.45
25	6	306	CLA	MG-NB	-2.18	2.01	2.05
25	b	606	CLA	CMC-C2C	-2.18	1.46	1.50
25	c	604	CLA	CMD-C2D	-2.18	1.46	1.50
25	p	317	CLA	MG-NB	-2.18	2.01	2.05
25	S	612	CLA	CMD-C2D	-2.18	1.46	1.50
25	c	612	CLA	CMB-C2B	-2.18	1.46	1.50
25	6	314	CLA	MG-NB	-2.18	2.01	2.05
25	n	306	CLA	MG-NB	-2.18	2.01	2.05
25	2	314	CLA	CHC-C1C	2.18	1.42	1.38
25	g	314	CLA	CHC-C1C	2.18	1.42	1.38
24	N	317	CHL	C1C-NC	-2.18	1.34	1.37
25	c	607	CLA	CMC-C2C	-2.18	1.46	1.50
25	Y	306	CLA	CMD-C2D	-2.18	1.46	1.50
25	A	607	CLA	CMB-C2B	-2.18	1.46	1.50
32	A	609	SQD	O2-C2	-2.18	1.37	1.43
25	8	305	CLA	CMD-C2D	-2.18	1.46	1.50
25	b	615	CLA	CMD-C2D	-2.18	1.46	1.50
25	3	307	CLA	MG-NB	-2.18	2.01	2.05
25	C	605	CLA	CMC-C2C	-2.18	1.46	1.50
25	C	612	CLA	CMC-C2C	-2.18	1.46	1.50
25	G	308	CLA	MG-NB	-2.18	2.01	2.05
25	u	317	CLA	CMD-C2D	-2.18	1.46	1.50
24	9	305	CHL	C1B-NB	-2.18	1.35	1.37
24	u	311	CHL	C1C-NC	-2.17	1.34	1.37
24	7	309	CHL	C1C-NC	-2.17	1.34	1.37
25	G	315	CLA	MG-NB	-2.17	2.01	2.05
25	C	610	CLA	CMC-C2C	-2.17	1.46	1.50
25	a	607	CLA	CMD-C2D	-2.17	1.46	1.50
25	6	307	CLA	CHC-C1C	2.17	1.42	1.38
30	A	601	LHG	O8-C23	2.17	1.39	1.33
24	1	305	CHL	C1C-NC	-2.17	1.34	1.37
24	u	312	CHL	C1B-NB	-2.17	1.35	1.37
24	q	308	CHL	CHB-C4A	-2.17	1.32	1.37
25	B	615	CLA	CMD-C2D	-2.17	1.46	1.50
25	C	611	CLA	CMC-C2C	-2.17	1.46	1.50
25	1	307	CLA	CMB-C2B	-2.17	1.46	1.50
25	2	316	CLA	MG-NB	-2.17	2.01	2.05
25	3	314	CLA	MG-NB	-2.17	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	304	CHL	C1C-NC	-2.17	1.34	1.37
25	q	306	CLA	CMB-C2B	-2.17	1.46	1.50
28	4	303	NEX	O24-C25	-2.17	1.43	1.46
28	7	304	NEX	O24-C25	-2.17	1.43	1.46
25	u	316	CLA	CHC-C1C	2.17	1.42	1.38
25	d	405	CLA	CMB-C2B	-2.17	1.46	1.50
24	4	305	CHL	C1C-NC	-2.17	1.34	1.37
25	7	308	CLA	MG-NB	-2.17	2.01	2.05
24	y	312	CHL	CHB-C4A	-2.17	1.32	1.37
25	3	315	CLA	MG-NB	-2.17	2.01	2.05
25	u	307	CLA	MG-NB	-2.17	2.01	2.05
25	3	314	CLA	CHC-C1C	2.17	1.42	1.38
24	1	310	CHL	C1C-NC	-2.17	1.34	1.37
24	4	304	CHL	C1C-NC	-2.17	1.34	1.37
25	S	610	CLA	CMD-C2D	-2.17	1.46	1.50
24	y	311	CHL	CHB-C4A	-2.17	1.32	1.37
24	4	309	CHL	C1C-NC	-2.17	1.34	1.37
24	g	306	CHL	C1B-NB	-2.17	1.35	1.37
25	8	314	CLA	CHC-C1C	2.17	1.42	1.38
25	B	616	CLA	CMD-C2D	-2.17	1.46	1.50
25	N	306	CLA	CHC-C1C	2.17	1.42	1.38
25	s	413	CLA	CMD-C2D	-2.17	1.46	1.50
28	5	304	NEX	O24-C25	-2.17	1.43	1.46
24	3	304	CHL	C1B-NB	-2.17	1.35	1.37
24	2	312	CHL	C4C-C3C	2.17	1.48	1.45
24	p	313	CHL	C4C-C3C	2.17	1.48	1.45
25	p	316	CLA	CMD-C2D	-2.17	1.46	1.50
24	2	305	CHL	C1B-NB	-2.17	1.35	1.37
24	N	309	CHL	C1B-NB	-2.17	1.35	1.37
24	4	310	CHL	C4C-C3C	2.17	1.48	1.45
25	9	315	CLA	CHC-C1C	2.17	1.42	1.38
39	D	406	PL9	C46-C44	-2.17	1.46	1.51
24	n	305	CHL	C1B-NB	-2.17	1.35	1.37
24	5	310	CHL	C1C-NC	-2.17	1.34	1.37
28	r	301	NEX	O24-C25	-2.17	1.43	1.46
24	n	309	CHL	C4C-C3C	2.17	1.48	1.45
24	3	312	CHL	C1C-NC	-2.17	1.34	1.37
24	6	311	CHL	C1C-NC	-2.17	1.34	1.37
25	B	609	CLA	CMD-C2D	-2.17	1.46	1.50
25	N	316	CLA	CHC-C1C	2.17	1.42	1.38
24	S	605	CHL	C1C-NC	-2.16	1.34	1.37
25	R	609	CLA	CMC-C2C	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	7	307	CLA	CMD-C2D	-2.16	1.46	1.50
24	p	305	CHL	C1B-NB	-2.16	1.35	1.37
25	Y	306	CLA	CMB-C2B	-2.16	1.46	1.50
24	N	304	CHL	C1B-NB	-2.16	1.35	1.37
24	g	310	CHL	C1B-NB	-2.16	1.35	1.37
25	4	314	CLA	CHC-C1C	2.16	1.42	1.38
24	Y	304	CHL	CHB-C4A	-2.16	1.32	1.37
25	B	610	CLA	CMC-C2C	-2.16	1.46	1.50
25	B	616	CLA	CMB-C2B	-2.16	1.46	1.50
25	b	610	CLA	CMC-C2C	-2.16	1.46	1.50
25	3	307	CLA	CHC-C1C	2.16	1.42	1.38
24	G	311	CHL	C1C-NC	-2.16	1.34	1.37
25	b	608	CLA	CMD-C2D	-2.16	1.46	1.50
24	6	312	CHL	C1C-NC	-2.16	1.34	1.37
25	6	315	CLA	MG-NB	-2.16	2.01	2.05
25	c	605	CLA	CMC-C2C	-2.16	1.46	1.50
24	y	313	CHL	CHB-C4A	-2.16	1.32	1.37
24	G	318	CHL	C1C-NC	-2.16	1.34	1.37
24	6	310	CHL	C1C-NC	-2.16	1.34	1.37
25	n	307	CLA	MG-NB	-2.16	2.01	2.05
25	R	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	p	314	CLA	CMB-C2B	-2.16	1.46	1.50
25	7	316	CLA	CMD-C2D	-2.16	1.46	1.50
24	7	313	CHL	C4C-C3C	2.16	1.48	1.45
39	d	406	PL9	C36-C34	-2.16	1.46	1.51
25	S	610	CLA	CMB-C2B	-2.16	1.46	1.50
25	C	606	CLA	CMC-C2C	-2.16	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.16	1.46	1.50
25	c	606	CLA	CMC-C2C	-2.16	1.46	1.50
24	R	605	CHL	C2C-C1C	2.16	1.49	1.44
28	G	304	NEX	O24-C25	-2.16	1.43	1.46
24	3	311	CHL	C1B-NB	-2.16	1.35	1.37
24	Y	304	CHL	C1B-NB	-2.16	1.35	1.37
24	N	309	CHL	C4C-C3C	2.16	1.48	1.45
24	3	317	CHL	C1C-NC	-2.16	1.34	1.37
25	7	314	CLA	CMB-C2B	-2.16	1.46	1.50
30	2	319	LHG	O7-C7	2.16	1.40	1.34
25	9	314	CLA	CHC-C1C	2.16	1.42	1.38
25	A	607	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	611	CLA	CMD-C2D	-2.16	1.46	1.50
24	R	607	CHL	C4C-C3C	2.16	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	314	CLA	CHC-C1C	2.16	1.42	1.38
24	4	311	CHL	C1C-NC	-2.16	1.34	1.37
25	R	613	CLA	CMB-C2B	-2.16	1.46	1.50
24	q	316	CHL	C2C-C1C	2.16	1.49	1.44
24	p	310	CHL	C4C-C3C	2.16	1.48	1.45
25	6	315	CLA	CHC-C1C	2.16	1.42	1.38
25	C	603	CLA	CMB-C2B	-2.16	1.46	1.50
25	7	315	CLA	CMB-C2B	-2.16	1.46	1.50
25	7	317	CLA	MG-NB	-2.16	2.01	2.05
24	g	311	CHL	C1C-NC	-2.16	1.34	1.37
25	s	412	CLA	CMB-C2B	-2.15	1.46	1.50
25	A	604	CLA	C1B-NB	-2.15	1.35	1.37
25	G	316	CLA	CHC-C1C	2.15	1.42	1.38
30	9	318	LHG	O7-C5	-2.15	1.41	1.46
24	q	308	CHL	C1B-C2B	2.15	1.48	1.43
28	r	317	NEX	O24-C25	-2.15	1.43	1.46
24	S	607	CHL	C1B-NB	-2.15	1.35	1.37
24	n	309	CHL	C1B-NB	-2.15	1.35	1.37
39	d	406	PL9	C16-C14	-2.15	1.46	1.51
30	c	617	LHG	O8-C23	2.15	1.39	1.33
25	s	411	CLA	CMD-C2D	-2.15	1.46	1.50
25	q	315	CLA	CHC-C1C	2.15	1.42	1.38
24	Y	310	CHL	CHB-C4A	-2.15	1.32	1.37
25	u	316	CLA	MG-NB	-2.15	2.01	2.05
25	b	615	CLA	CMB-C2B	-2.15	1.46	1.50
29	1	301	0UR	C19-C18	2.15	1.53	1.50
25	n	316	CLA	CHC-C1C	2.15	1.42	1.38
24	n	308	CHL	C1C-NC	-2.15	1.34	1.37
25	6	307	CLA	MG-NB	-2.15	2.01	2.05
25	B	608	CLA	CMD-C2D	-2.15	1.46	1.50
25	Y	316	CLA	CMB-C2B	-2.15	1.46	1.50
25	6	314	CLA	CHC-C1C	2.15	1.42	1.38
25	g	315	CLA	MG-NB	-2.15	2.01	2.05
25	8	312	CLA	CMD-C2D	-2.15	1.46	1.50
24	7	318	CHL	C1C-NC	-2.15	1.34	1.37
25	C	609	CLA	C1B-C2B	2.15	1.48	1.43
31	s	416	8CT	C14-C15	2.15	1.40	1.34
25	N	315	CLA	MG-NB	-2.15	2.01	2.05
25	3	316	CLA	CHC-C1C	2.15	1.42	1.38
28	9	319	NEX	O24-C25	-2.15	1.43	1.46
24	u	312	CHL	C4C-C3C	2.15	1.48	1.45
24	r	308	CHL	C4C-C3C	2.15	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	306	CLA	MG-NB	-2.15	2.01	2.05
25	b	607	CLA	CMD-C2D	-2.15	1.46	1.50
24	N	305	CHL	C2C-C1C	2.15	1.49	1.44
24	N	311	CHL	C1C-NC	-2.15	1.34	1.37
24	g	306	CHL	C1C-NC	-2.15	1.34	1.37
25	4	307	CLA	CMB-C2B	-2.15	1.46	1.50
25	u	308	CLA	CHC-C1C	2.15	1.42	1.38
24	r	306	CHL	C4C-C3C	2.15	1.48	1.45
24	u	313	CHL	C1C-NC	-2.15	1.34	1.37
25	N	313	CLA	MG-NB	-2.15	2.01	2.05
25	b	616	CLA	CMD-C2D	-2.15	1.46	1.50
25	c	601	CLA	CMC-C2C	-2.15	1.46	1.50
24	9	305	CHL	C1C-NC	-2.15	1.34	1.37
30	a	601	LHG	O8-C23	2.15	1.39	1.33
28	u	304	NEX	O24-C25	-2.14	1.43	1.46
25	y	317	CLA	CMB-C2B	-2.14	1.46	1.50
24	9	311	CHL	C2C-C1C	2.14	1.49	1.44
30	C	617	LHG	O8-C23	2.14	1.39	1.33
25	Y	316	CLA	CMC-C2C	-2.14	1.46	1.50
24	g	310	CHL	C1C-NC	-2.14	1.34	1.37
24	n	304	CHL	C1C-NC	-2.14	1.34	1.37
25	1	315	CLA	CHC-C1C	2.14	1.42	1.38
25	9	306	CLA	CHC-C1C	2.14	1.42	1.38
25	C	611	CLA	CMB-C2B	-2.14	1.46	1.50
24	S	607	CHL	C4C-C3C	2.14	1.48	1.45
30	5	319	LHG	O7-C7	2.14	1.40	1.34
24	G	305	CHL	C1C-NC	-2.14	1.34	1.37
25	r	312	CLA	CHC-C1C	2.14	1.42	1.38
31	V	401	8CT	C33-C32	-2.14	1.44	1.50
25	N	314	CLA	MG-NB	-2.14	2.01	2.05
24	y	305	CHL	CHB-C4A	-2.14	1.32	1.37
24	N	304	CHL	C1C-NC	-2.14	1.34	1.37
24	y	310	CHL	C1B-C2B	2.14	1.48	1.43
25	7	316	CLA	CMC-C2C	-2.14	1.46	1.50
28	R	616	NEX	O24-C25	-2.14	1.43	1.46
25	6	316	CLA	MG-NB	-2.14	2.01	2.05
24	8	303	CHL	C4C-C3C	2.14	1.48	1.45
25	c	608	CLA	C1B-C2B	2.14	1.48	1.43
25	Y	313	CLA	CMC-C2C	-2.14	1.46	1.50
25	s	411	CLA	CMB-C2B	-2.14	1.46	1.50
25	7	317	CLA	CMB-C2B	-2.14	1.46	1.50
24	n	317	CHL	C1C-NC	-2.14	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	601	CLA	CMC-C2C	-2.14	1.46	1.50
25	y	307	CLA	CMD-C2D	-2.14	1.46	1.50
25	c	612	CLA	CMC-C2C	-2.14	1.46	1.50
25	R	609	CLA	CMD-C2D	-2.14	1.46	1.50
25	5	315	CLA	CMB-C2B	-2.14	1.46	1.50
25	S	611	CLA	CMB-C2B	-2.14	1.46	1.50
25	s	413	CLA	CMB-C2B	-2.14	1.46	1.50
25	c	604	CLA	CMB-C2B	-2.14	1.46	1.50
25	N	316	CLA	MG-NB	-2.14	2.01	2.05
25	p	315	CLA	CMD-C2D	-2.14	1.46	1.50
25	7	315	CLA	CMD-C2D	-2.14	1.46	1.50
25	Y	314	CLA	CMC-C2C	-2.13	1.46	1.50
24	1	304	CHL	C1C-NC	-2.13	1.34	1.37
24	6	317	CHL	C1C-NC	-2.13	1.34	1.37
24	9	311	CHL	C4C-C3C	2.13	1.48	1.45
30	y	319	LHG	O7-C7	2.13	1.40	1.34
24	s	408	CHL	C1B-NB	-2.13	1.35	1.37
25	u	307	CLA	CHC-C1C	2.13	1.42	1.38
25	n	315	CLA	MG-NB	-2.13	2.01	2.05
25	a	604	CLA	C1B-NB	-2.13	1.35	1.37
25	C	616	CLA	CMC-C2C	-2.13	1.46	1.50
25	C	608	CLA	C1B-C2B	2.13	1.48	1.43
31	T	101	8CT	C33-C32	-2.13	1.44	1.50
25	R	612	CLA	CMD-C2D	-2.13	1.46	1.50
24	9	310	CHL	C1C-NC	-2.13	1.34	1.37
25	u	308	CLA	MG-NB	-2.13	2.01	2.05
24	Y	311	CHL	CHB-C4A	-2.13	1.32	1.37
24	s	407	CHL	C4C-C3C	2.13	1.48	1.45
25	B	602	CLA	CMB-C2B	-2.13	1.46	1.50
25	G	308	CLA	CHC-C1C	2.13	1.42	1.38
25	B	615	CLA	CMB-C2B	-2.13	1.46	1.50
28	S	617	NEX	O24-C25	-2.13	1.43	1.46
25	N	314	CLA	CHC-C1C	2.13	1.42	1.38
24	3	308	CHL	C2C-C1C	2.13	1.49	1.44
25	c	609	CLA	C1B-C2B	2.13	1.48	1.43
25	y	317	CLA	CMC-C2C	-2.13	1.46	1.50
24	2	311	CHL	C1C-NC	-2.13	1.34	1.37
24	4	310	CHL	C1C-NC	-2.13	1.34	1.37
25	A	610	CLA	CMD-C2D	-2.13	1.46	1.50
24	G	305	CHL	C4C-C3C	2.13	1.48	1.45
25	b	612	CLA	CMC-C2C	-2.13	1.46	1.50
25	1	315	CLA	MG-NB	-2.13	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	306	CLA	CHC-C1C	2.13	1.42	1.38
25	a	610	CLA	CMD-C2D	-2.13	1.46	1.50
25	u	317	CLA	MG-NB	-2.13	2.01	2.05
25	r	313	CLA	MG-NB	-2.13	2.01	2.05
28	y	304	NEX	O24-C25	-2.13	1.43	1.46
25	S	609	CLA	CMD-C2D	-2.13	1.46	1.50
25	n	313	CLA	MG-NB	-2.13	2.01	2.05
25	9	307	CLA	CHC-C1C	2.13	1.42	1.38
25	2	315	CLA	CMB-C2B	-2.13	1.46	1.50
25	b	601	CLA	CMD-C2D	-2.13	1.46	1.50
24	7	305	CHL	C1C-NC	-2.13	1.34	1.37
25	g	316	CLA	CHC-C1C	2.13	1.42	1.38
25	8	313	CLA	CMD-C2D	-2.13	1.46	1.50
25	C	604	CLA	CMC-C2C	-2.13	1.46	1.50
25	C	607	CLA	CMC-C2C	-2.13	1.46	1.50
25	c	604	CLA	CMC-C2C	-2.13	1.46	1.50
24	3	310	CHL	C1C-NC	-2.13	1.34	1.37
24	Y	305	CHL	C1B-C2B	2.13	1.48	1.43
25	2	315	CLA	CMD-C2D	-2.12	1.46	1.50
24	9	308	CHL	C1C-NC	-2.12	1.34	1.37
24	y	313	CHL	C1B-C2B	2.12	1.48	1.43
30	D	408	LHG	O7-C7	2.12	1.40	1.34
25	p	316	CLA	CMC-C2C	-2.12	1.46	1.50
24	u	312	CHL	C2C-C1C	2.12	1.49	1.44
25	R	613	CLA	CHC-C1C	2.12	1.42	1.38
28	n	303	NEX	O24-C25	-2.12	1.43	1.46
25	Y	307	CLA	CMB-C2B	-2.12	1.46	1.50
26	u	303	0IE	C13-C12	-2.12	1.41	1.45
24	6	308	CHL	C1B-NB	-2.12	1.35	1.37
28	2	304	NEX	O24-C25	-2.12	1.43	1.46
25	R	611	CLA	CHC-C1C	2.12	1.42	1.38
31	v	401	8CT	C33-C32	-2.12	1.44	1.50
25	g	308	CLA	CHC-C1C	2.12	1.42	1.38
25	y	314	CLA	CMC-C2C	-2.12	1.46	1.50
25	N	315	CLA	CHC-C1C	2.12	1.42	1.38
25	8	306	CLA	CMD-C2D	-2.12	1.46	1.50
25	q	306	CLA	CMD-C2D	-2.12	1.46	1.50
25	9	307	CLA	MG-NB	-2.12	2.01	2.05
25	s	404	CLA	CMD-C2D	-2.12	1.46	1.50
25	G	307	CLA	CHC-C1C	2.12	1.42	1.38
25	2	316	CLA	CMD-C2D	-2.12	1.46	1.50
24	G	312	CHL	C1C-NC	-2.12	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	605	CHL	C1B-NB	-2.12	1.35	1.37
28	3	318	NEX	O24-C25	-2.12	1.43	1.46
25	g	308	CLA	MG-NB	-2.12	2.01	2.05
24	6	308	CHL	C1C-NC	-2.12	1.34	1.37
24	4	308	CHL	C1C-NC	-2.12	1.34	1.37
24	y	318	CHL	CHB-C4A	-2.12	1.32	1.37
25	5	315	CLA	CMD-C2D	-2.12	1.46	1.50
25	p	315	CLA	CMB-C2B	-2.12	1.46	1.50
24	q	311	CHL	C4C-C3C	2.12	1.48	1.45
25	4	315	CLA	MG-NB	-2.12	2.01	2.05
28	6	303	NEX	O24-C25	-2.12	1.43	1.46
24	5	312	CHL	C1C-NC	-2.12	1.34	1.37
24	G	312	CHL	C1B-NB	-2.12	1.35	1.37
39	D	406	PL9	C16-C14	-2.12	1.46	1.51
24	8	310	CHL	C4C-C3C	2.12	1.48	1.45
24	r	308	CHL	CHB-C4A	-2.12	1.32	1.37
25	Y	307	CLA	CMD-C2D	-2.12	1.46	1.50
25	G	307	CLA	MG-NB	-2.12	2.01	2.05
25	g	307	CLA	MG-NB	-2.12	2.01	2.05
25	S	612	CLA	CMB-C2B	-2.12	1.46	1.50
25	C	604	CLA	CMB-C2B	-2.12	1.46	1.50
24	R	602	CHL	CHB-C4A	-2.12	1.32	1.37
25	c	603	CLA	CMB-C2B	-2.12	1.46	1.50
25	c	611	CLA	CMD-C2D	-2.12	1.46	1.50
25	c	616	CLA	CMC-C2C	-2.12	1.46	1.50
25	4	316	CLA	MG-NB	-2.11	2.01	2.05
24	8	304	CHL	C4C-C3C	2.11	1.48	1.45
25	R	604	CLA	CMD-C2D	-2.11	1.46	1.50
25	C	603	CLA	CMC-C2C	-2.11	1.46	1.50
25	r	313	CLA	CMD-C2D	-2.11	1.46	1.50
24	G	310	CHL	C1B-NB	-2.11	1.35	1.37
24	Y	312	CHL	C1B-C2B	2.11	1.48	1.43
28	N	303	NEX	O24-C25	-2.11	1.43	1.46
25	a	610	CLA	MG-NB	-2.11	2.01	2.05
25	5	308	CLA	CHC-C1C	2.11	1.42	1.38
25	A	605	CLA	CMC-C2C	-2.11	1.46	1.50
25	a	607	CLA	CMC-C2C	-2.11	1.46	1.50
25	1	313	CLA	MG-NB	-2.11	2.01	2.05
25	N	307	CLA	MG-NB	-2.11	2.01	2.05
25	5	307	CLA	CMD-C2D	-2.11	1.46	1.50
25	y	308	CLA	CMB-C2B	-2.11	1.46	1.50
31	S	615	8CT	C14-C15	2.11	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	304	CHL	C1C-NC	-2.11	1.34	1.37
25	C	611	CLA	CMD-C2D	-2.11	1.46	1.50
24	y	306	CHL	C1B-C2B	2.11	1.48	1.43
24	1	310	CHL	C2C-C1C	2.11	1.49	1.44
25	c	601	CLA	C1B-NB	-2.11	1.35	1.37
25	b	612	CLA	C1B-C2B	2.11	1.48	1.43
31	D	410	8CT	C33-C32	-2.11	1.44	1.50
25	p	317	CLA	CMD-C2D	-2.11	1.46	1.50
25	S	616	CLA	CHC-C1C	2.11	1.42	1.38
29	4	301	0UR	C19-C18	2.11	1.53	1.50
30	D	408	LHG	O8-C23	2.11	1.39	1.33
25	3	315	CLA	CHC-C1C	2.11	1.42	1.38
24	3	317	CHL	C1B-NB	-2.11	1.35	1.37
24	p	312	CHL	C1B-NB	-2.11	1.35	1.37
24	R	605	CHL	CHB-C4A	-2.11	1.32	1.37
25	B	601	CLA	CMB-C2B	-2.11	1.46	1.50
25	5	307	CLA	CMB-C2B	-2.11	1.46	1.50
25	6	313	CLA	MG-NB	-2.11	2.01	2.05
25	7	317	CLA	CHC-C1C	2.11	1.42	1.38
24	Y	319	CHL	CHB-C4A	-2.11	1.32	1.37
39	d	406	PL9	C46-C44	-2.11	1.46	1.51
25	B	601	CLA	CMD-C2D	-2.10	1.46	1.50
24	g	305	CHL	C4C-C3C	2.10	1.48	1.45
24	8	315	CHL	C2C-C1C	2.10	1.49	1.44
25	a	604	CLA	CMC-C2C	-2.10	1.46	1.50
24	6	317	CHL	C1B-NB	-2.10	1.35	1.37
25	y	316	CLA	MG-ND	-2.10	2.01	2.05
24	Y	317	CHL	CHB-C4A	-2.10	1.32	1.37
31	t	101	8CT	C33-C32	-2.10	1.44	1.50
24	7	306	CHL	C1B-C2B	2.10	1.48	1.43
24	q	304	CHL	C1B-C2B	2.10	1.48	1.43
25	q	313	CLA	CMD-C2D	-2.10	1.46	1.50
25	b	603	CLA	MG-ND	-2.10	2.01	2.05
24	n	311	CHL	C1C-NC	-2.10	1.34	1.37
25	5	316	CLA	CMD-C2D	-2.10	1.46	1.50
25	2	308	CLA	CHC-C1C	2.10	1.42	1.38
25	9	315	CLA	MG-NB	-2.10	2.01	2.05
25	S	610	CLA	CMC-C2C	-2.10	1.46	1.50
24	p	306	CHL	C1B-C2B	2.10	1.48	1.43
25	R	612	CLA	MG-NB	-2.10	2.01	2.05
25	r	312	CLA	CMB-C2B	-2.10	1.46	1.50
25	n	314	CLA	MG-NB	-2.10	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	CHB-C4A	-2.10	1.32	1.37
25	3	306	CLA	CHC-C1C	2.10	1.42	1.38
25	6	316	CLA	CHC-C1C	2.10	1.42	1.38
24	n	305	CHL	C2C-C1C	2.10	1.49	1.44
24	9	309	CHL	C2C-C1C	2.10	1.49	1.44
25	S	603	CLA	CMD-C2D	-2.10	1.46	1.50
25	n	316	CLA	MG-NB	-2.10	2.01	2.05
28	s	401	NEX	O24-C25	-2.10	1.43	1.46
24	G	309	CHL	C1C-NC	-2.10	1.34	1.37
25	S	612	CLA	CMC-C2C	-2.10	1.46	1.50
25	b	607	CLA	CMC-C2C	-2.10	1.46	1.50
30	D	407	LHG	O8-C23	2.10	1.39	1.33
25	4	314	CLA	MG-NB	-2.10	2.01	2.05
24	3	305	CHL	C4C-C3C	2.10	1.48	1.45
24	q	310	CHL	CHB-C4A	-2.10	1.32	1.37
25	y	308	CLA	CMD-C2D	-2.10	1.46	1.50
24	6	305	CHL	C4C-C3C	2.10	1.48	1.45
25	r	314	CLA	CMB-C2B	-2.10	1.46	1.50
25	3	316	CLA	MG-NB	-2.10	2.01	2.05
24	r	303	CHL	CHB-C4A	-2.10	1.32	1.37
24	N	305	CHL	C1C-NC	-2.10	1.34	1.37
24	q	316	CHL	C1C-NC	-2.10	1.34	1.37
24	9	308	CHL	C2C-C1C	2.10	1.49	1.44
25	B	603	CLA	MG-ND	-2.10	2.01	2.05
25	N	315	CLA	CMD-C2D	-2.10	1.46	1.50
25	r	304	CLA	CMD-C2D	-2.10	1.46	1.50
24	N	310	CHL	C1C-NC	-2.10	1.34	1.37
25	y	315	CLA	CMC-C2C	-2.10	1.46	1.50
25	A	604	CLA	CMC-C2C	-2.10	1.46	1.50
25	n	315	CLA	CHC-C1C	2.10	1.42	1.38
39	d	406	PL9	C7-C8	-2.10	1.47	1.50
25	u	314	CLA	MG-NB	-2.10	2.01	2.05
24	1	317	CHL	C1B-NB	-2.10	1.35	1.37
24	S	605	CHL	C4C-C3C	2.09	1.48	1.45
25	A	603	CLA	CMB-C2B	-2.09	1.46	1.50
25	a	603	CLA	CMB-C2B	-2.09	1.46	1.50
25	R	610	CLA	CHC-C1C	2.09	1.42	1.38
25	B	607	CLA	CMD-C2D	-2.09	1.46	1.50
24	N	305	CHL	C4C-C3C	2.09	1.48	1.45
25	Y	307	CLA	CHC-C1C	2.09	1.42	1.38
25	B	607	CLA	CMC-C2C	-2.09	1.46	1.50
24	9	311	CHL	C1C-NC	-2.09	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	310	CHL	C2C-C1C	2.09	1.49	1.44
24	q	309	CHL	CHB-C4A	-2.09	1.32	1.37
30	4	318	LHG	P-O6	2.09	1.67	1.59
24	n	310	CHL	C1C-NC	-2.09	1.34	1.37
24	p	305	CHL	CHB-C4A	-2.09	1.32	1.37
25	2	307	CLA	CMD-C2D	-2.09	1.46	1.50
25	S	603	CLA	CMB-C2B	-2.09	1.46	1.50
25	q	314	CLA	CMD-C2D	-2.09	1.46	1.50
25	b	601	CLA	CMB-C2B	-2.09	1.46	1.50
24	1	305	CHL	C4C-C3C	2.09	1.48	1.45
25	1	316	CLA	MG-NB	-2.09	2.01	2.05
25	b	607	CLA	CHC-C1C	2.09	1.42	1.38
25	8	314	CLA	CMD-C2D	-2.09	1.46	1.50
24	s	406	CHL	C4C-C3C	2.09	1.48	1.45
25	4	306	CLA	CHC-C1C	2.09	1.42	1.38
24	p	309	CHL	C1C-NC	-2.09	1.34	1.37
25	n	315	CLA	CMC-C2C	-2.09	1.46	1.50
24	g	312	CHL	C1C-NC	-2.09	1.34	1.37
25	G	316	CLA	CMD-C2D	-2.09	1.46	1.50
24	Y	309	CHL	C1B-C2B	2.09	1.48	1.43
24	6	308	CHL	C2C-C1C	2.09	1.49	1.44
24	9	304	CHL	C1B-NB	-2.09	1.35	1.37
25	7	308	CLA	CHC-C1C	2.09	1.42	1.38
24	u	309	CHL	C2C-C1C	2.09	1.49	1.44
24	p	305	CHL	C1C-NC	-2.09	1.34	1.37
25	s	410	CLA	CMB-C2B	-2.09	1.46	1.50
25	s	413	CLA	CMC-C2C	-2.09	1.46	1.50
24	y	313	CHL	C4C-C3C	2.09	1.48	1.45
25	7	317	CLA	CMD-C2D	-2.09	1.46	1.50
25	7	308	CLA	CMB-C2B	-2.09	1.46	1.50
25	C	607	CLA	MG-ND	-2.09	2.01	2.05
24	G	309	CHL	C2C-C1C	2.09	1.49	1.44
25	3	313	CLA	MG-NB	-2.09	2.01	2.05
25	3	315	CLA	CMC-C2C	-2.09	1.46	1.50
25	Y	307	CLA	CMC-C2C	-2.09	1.46	1.50
25	8	311	CLA	CMD-C2D	-2.09	1.46	1.50
25	n	315	CLA	CMD-C2D	-2.09	1.46	1.50
25	b	604	CLA	CMC-C2C	-2.09	1.46	1.50
25	g	314	CLA	MG-NB	-2.09	2.01	2.05
25	7	315	CLA	CHC-C1C	2.09	1.42	1.38
25	G	317	CLA	CMD-C2D	-2.08	1.46	1.50
25	2	307	CLA	CHC-C1C	2.08	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	404	CLA	CMB-C2B	-2.08	1.46	1.50
37	c	619	DGD	O2G-C2G	-2.08	1.41	1.46
25	4	315	CLA	CHC-C1C	2.08	1.42	1.38
25	Y	306	CLA	CMC-C2C	-2.08	1.46	1.50
25	q	312	CLA	CMD-C2D	-2.08	1.46	1.50
24	s	407	CHL	CHB-C4A	-2.08	1.32	1.37
25	S	604	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	608	CLA	CMC-C2C	-2.08	1.46	1.50
25	9	314	CLA	MG-NB	-2.08	2.01	2.05
24	2	306	CHL	CHB-C4A	-2.08	1.32	1.37
24	4	317	CHL	C2C-C1C	2.08	1.49	1.44
25	r	312	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	607	CLA	MG-ND	-2.08	2.01	2.05
25	s	410	CLA	CMD-C2D	-2.08	1.46	1.50
25	p	308	CLA	CMD-C2D	-2.08	1.46	1.50
24	G	306	CHL	C1C-NC	-2.08	1.34	1.37
25	s	412	CLA	CMC-C2C	-2.08	1.46	1.50
25	4	306	CLA	CMD-C2D	-2.08	1.46	1.50
24	n	305	CHL	C1C-NC	-2.08	1.34	1.37
24	2	312	CHL	C1B-NB	-2.08	1.35	1.37
25	r	311	CLA	CHC-C1C	2.08	1.42	1.38
24	R	608	CHL	C4C-C3C	2.08	1.48	1.45
25	S	609	CLA	CMB-C2B	-2.08	1.46	1.50
25	b	602	CLA	CMB-C2B	-2.08	1.46	1.50
30	Y	318	LHG	O7-C7	2.08	1.40	1.34
32	A	609	SQD	O4-C4	-2.08	1.38	1.43
25	q	312	CLA	CHC-C1C	2.08	1.42	1.38
25	b	614	CLA	CMC-C2C	-2.08	1.46	1.50
25	D	405	CLA	CMC-C2C	-2.08	1.46	1.50
25	9	316	CLA	MG-NB	-2.08	2.01	2.05
32	A	609	SQD	O3-C3	-2.08	1.38	1.43
25	S	611	CLA	CHC-C1C	2.08	1.42	1.38
25	5	317	CLA	CMD-C2D	-2.08	1.46	1.50
24	4	305	CHL	C4C-C3C	2.08	1.48	1.45
24	N	311	CHL	CHB-C4A	-2.08	1.32	1.37
25	S	611	CLA	CMC-C2C	-2.08	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.08	1.46	1.50
24	2	312	CHL	C1C-NC	-2.08	1.34	1.37
25	5	314	CLA	CMD-C2D	-2.08	1.46	1.50
24	6	311	CHL	C1B-NB	-2.08	1.35	1.37
24	8	310	CHL	C1B-C2B	2.08	1.48	1.43
25	B	612	CLA	C1B-C2B	2.08	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	314	CLA	CHC-C1C	2.07	1.42	1.38
25	G	314	CLA	MG-NB	-2.07	2.01	2.05
25	4	313	CLA	MG-NB	-2.07	2.01	2.05
24	7	312	CHL	C1B-NB	-2.07	1.35	1.37
25	C	616	CLA	C1B-NB	-2.07	1.35	1.37
25	S	616	CLA	CMD-C2D	-2.07	1.46	1.50
25	6	306	CLA	CHC-C1C	2.07	1.42	1.38
25	p	316	CLA	CHC-C1C	2.07	1.42	1.38
25	c	605	CLA	CHC-C1C	2.07	1.42	1.38
25	s	410	CLA	CHC-C1C	2.07	1.42	1.38
24	8	308	CHL	C1B-C2B	2.07	1.48	1.43
30	d	407	LHG	O8-C23	2.07	1.39	1.33
24	1	308	CHL	C1C-NC	-2.07	1.34	1.37
25	C	601	CLA	C1B-NB	-2.07	1.35	1.37
25	p	317	CLA	CMB-C2B	-2.07	1.46	1.50
25	Y	313	CLA	CHC-C1C	2.07	1.42	1.38
32	a	609	SQD	O4-C4	-2.07	1.38	1.43
24	9	310	CHL	C2C-C1C	2.07	1.49	1.44
25	p	308	CLA	CHC-C1C	2.07	1.42	1.38
25	r	314	CLA	CHC-C1C	2.07	1.42	1.38
31	d	410	8CT	C33-C32	-2.07	1.44	1.50
25	R	611	CLA	CMB-C2B	-2.07	1.46	1.50
24	8	304	CHL	C1B-C2B	2.07	1.48	1.43
24	r	309	CHL	C4C-C3C	2.07	1.48	1.45
25	y	308	CLA	CHC-C1C	2.07	1.42	1.38
25	p	314	CLA	CHC-C1C	2.07	1.42	1.38
24	u	306	CHL	CHB-C4A	-2.07	1.32	1.37
25	C	606	CLA	MG-ND	-2.07	2.01	2.05
25	c	606	CLA	MG-ND	-2.07	2.01	2.05
25	Y	316	CLA	CHC-C1C	2.07	1.42	1.38
24	g	309	CHL	C1C-NC	-2.07	1.34	1.37
24	u	318	CHL	C1C-NC	-2.07	1.34	1.37
24	7	305	CHL	CHB-C4A	-2.07	1.32	1.37
30	1	318	LHG	P-O6	2.07	1.67	1.59
25	C	608	CLA	MG-ND	-2.07	2.01	2.05
25	7	314	CLA	CMD-C2D	-2.07	1.46	1.50
25	N	315	CLA	CMC-C2C	-2.07	1.46	1.50
25	7	308	CLA	CMD-C2D	-2.07	1.46	1.50
30	a	612	LHG	O7-C7	2.07	1.40	1.34
25	R	611	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	614	CLA	CMC-C2C	-2.07	1.46	1.50
25	q	315	CLA	CMD-C2D	-2.07	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	317	CHL	C2C-C1C	2.07	1.49	1.44
24	S	606	CHL	C4C-C3C	2.07	1.48	1.45
25	3	315	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	606	CLA	CMB-C2B	-2.07	1.46	1.50
25	c	610	CLA	CHC-C1C	2.07	1.42	1.38
24	u	311	CHL	C2C-C1C	2.07	1.49	1.44
25	n	307	CLA	CMD-C2D	-2.07	1.46	1.50
25	r	305	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	603	CLA	C1B-NB	-2.07	1.35	1.37
25	G	315	CLA	CMD-C2D	-2.07	1.46	1.50
25	g	316	CLA	CMD-C2D	-2.07	1.46	1.50
25	r	313	CLA	CMB-C2B	-2.07	1.46	1.50
25	A	610	CLA	MG-NB	-2.07	2.01	2.05
25	c	601	CLA	CMB-C2B	-2.07	1.46	1.50
24	u	309	CHL	C1C-NC	-2.07	1.34	1.37
25	B	604	CLA	CMC-C2C	-2.07	1.46	1.50
25	S	609	CLA	CMC-C2C	-2.07	1.46	1.50
25	4	313	CLA	CMD-C2D	-2.07	1.46	1.50
24	1	311	CHL	CHB-C4A	-2.07	1.32	1.37
24	g	309	CHL	C2C-C1C	2.07	1.49	1.44
25	7	316	CLA	CMB-C2B	-2.07	1.46	1.50
24	q	304	CHL	C4C-C3C	2.07	1.48	1.45
25	p	308	CLA	CMB-C2B	-2.07	1.46	1.50
25	b	613	CLA	CHC-C1C	2.06	1.42	1.38
24	u	306	CHL	C1C-NC	-2.06	1.34	1.37
25	d	405	CLA	CMC-C2C	-2.06	1.46	1.50
24	6	311	CHL	C2C-C1C	2.06	1.49	1.44
25	b	613	CLA	CMC-C2C	-2.06	1.46	1.50
25	7	317	CLA	CMC-C2C	-2.06	1.46	1.50
32	D	409	SQD	O3-C3	-2.06	1.38	1.43
25	p	317	CLA	CHC-C1C	2.06	1.42	1.38
25	b	601	CLA	CHC-C1C	2.06	1.42	1.38
25	s	412	CLA	CHC-C1C	2.06	1.42	1.38
25	2	307	CLA	CMB-C2B	-2.06	1.46	1.50
25	5	307	CLA	CHC-C1C	2.06	1.42	1.38
25	C	601	CLA	CMB-C2B	-2.06	1.46	1.50
25	u	315	CLA	MG-NB	-2.06	2.01	2.05
30	A	612	LHG	O7-C7	2.06	1.40	1.34
24	n	311	CHL	CHB-C4A	-2.06	1.32	1.37
24	8	307	CHL	C4C-C3C	2.06	1.48	1.45
24	S	606	CHL	CHB-C4A	-2.06	1.32	1.37
25	1	306	CLA	CHC-C1C	2.06	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	315	CLA	CHC-C1C	2.06	1.42	1.38
25	B	607	CLA	CHC-C1C	2.06	1.42	1.38
25	s	417	CLA	CMB-C2B	-2.06	1.46	1.50
24	G	306	CHL	CHB-C4A	-2.06	1.32	1.37
25	4	307	CLA	CHC-C1C	2.06	1.42	1.38
24	s	414	CHL	CHB-C4A	-2.06	1.32	1.37
25	a	605	CLA	CMC-C2C	-2.06	1.46	1.50
25	B	612	CLA	C1B-NB	-2.06	1.35	1.37
30	9	318	LHG	P-O6	2.06	1.67	1.59
24	3	304	CHL	CHB-C4A	-2.06	1.32	1.37
25	2	314	CLA	CMC-C2C	-2.06	1.46	1.50
25	1	307	CLA	CHC-C1C	2.06	1.42	1.38
25	1	314	CLA	MG-NB	-2.06	2.01	2.05
25	S	616	CLA	CMB-C2B	-2.06	1.46	1.50
24	S	613	CHL	CHB-C4A	-2.06	1.32	1.37
25	B	602	CLA	CHC-C1C	2.06	1.42	1.38
32	a	609	SQD	O3-C3	-2.06	1.38	1.43
32	d	409	SQD	O4-C4	-2.06	1.38	1.43
25	9	307	CLA	CMB-C2B	-2.06	1.46	1.50
25	N	306	CLA	CMD-C2D	-2.06	1.46	1.50
25	5	314	CLA	CMB-C2B	-2.06	1.46	1.50
25	2	317	CLA	CMD-C2D	-2.05	1.46	1.50
25	p	314	CLA	CMD-C2D	-2.05	1.46	1.50
25	C	602	CLA	C1B-NB	-2.05	1.35	1.37
24	G	312	CHL	C2C-C1C	2.05	1.49	1.44
25	g	315	CLA	CMD-C2D	-2.05	1.46	1.50
25	y	307	CLA	CMC-C2C	-2.05	1.46	1.50
25	9	313	CLA	MG-NB	-2.05	2.01	2.05
25	6	315	CLA	CMD-C2D	-2.05	1.46	1.50
25	p	316	CLA	CMB-C2B	-2.05	1.46	1.50
25	8	311	CLA	CHC-C1C	2.05	1.42	1.38
32	d	409	SQD	O3-C3	-2.05	1.38	1.43
25	c	607	CLA	C1B-NB	-2.05	1.35	1.37
24	q	311	CHL	C1B-C2B	2.05	1.48	1.43
24	3	305	CHL	C1C-NC	-2.05	1.34	1.37
24	3	308	CHL	C1C-NC	-2.05	1.34	1.37
25	5	314	CLA	CMC-C2C	-2.05	1.46	1.50
25	p	307	CLA	CMB-C2B	-2.05	1.46	1.50
25	R	611	CLA	CMC-C2C	-2.05	1.46	1.50
25	A	607	CLA	CMC-C2C	-2.05	1.46	1.50
24	5	306	CHL	CHB-C4A	-2.05	1.32	1.37
25	c	603	CLA	CMC-C2C	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	q	314	CLA	CMC-C2C	-2.05	1.46	1.50
25	s	405	CLA	CMD-C2D	-2.05	1.46	1.50
25	3	306	CLA	CMD-C2D	-2.05	1.46	1.50
25	5	317	CLA	CHC-C1C	2.05	1.42	1.38
25	b	603	CLA	C1B-NB	-2.05	1.35	1.37
25	s	413	CLA	CHC-C1C	2.05	1.42	1.38
32	B	618	SQD	O3-C3	-2.05	1.38	1.43
24	r	306	CHL	C1C-NC	-2.05	1.34	1.37
25	b	605	CLA	CMC-C2C	-2.05	1.46	1.50
24	g	312	CHL	C2C-C1C	2.05	1.49	1.44
25	u	316	CLA	CMD-C2D	-2.05	1.46	1.50
24	2	312	CHL	CHB-C4A	-2.05	1.32	1.37
24	S	602	CHL	CHB-C4A	-2.05	1.32	1.37
25	N	307	CLA	CMD-C2D	-2.05	1.46	1.50
24	n	305	CHL	C4C-C3C	2.05	1.48	1.45
25	g	317	CLA	CMD-C2D	-2.05	1.46	1.50
25	s	417	CLA	CMD-C2D	-2.05	1.46	1.50
25	n	314	CLA	CMD-C2D	-2.05	1.46	1.50
25	N	307	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	606	CLA	CMB-C2B	-2.05	1.46	1.50
24	S	607	CHL	CHB-C4A	-2.05	1.32	1.37
25	3	316	CLA	CMC-C2C	-2.05	1.46	1.50
25	G	316	CLA	CMC-C2C	-2.05	1.46	1.50
25	7	307	CLA	CMB-C2B	-2.05	1.46	1.50
24	4	311	CHL	CHB-C4A	-2.05	1.32	1.37
24	5	310	CHL	CHB-C4A	-2.05	1.32	1.37
24	s	408	CHL	CHB-C4A	-2.05	1.32	1.37
24	n	311	CHL	C2C-C1C	2.04	1.49	1.44
24	R	605	CHL	C4C-C3C	2.04	1.48	1.45
24	p	305	CHL	C4C-C3C	2.04	1.48	1.45
25	9	316	CLA	CMD-C2D	-2.04	1.46	1.50
24	1	308	CHL	C2C-C1C	2.04	1.49	1.44
25	8	311	CLA	CMC-C2C	-2.04	1.46	1.50
24	1	317	CHL	C1C-NC	-2.04	1.34	1.37
25	B	612	CLA	CMC-C2C	-2.04	1.46	1.50
24	5	306	CHL	C4C-C3C	2.04	1.48	1.45
25	r	312	CLA	CMC-C2C	-2.04	1.46	1.50
25	G	316	CLA	CMB-C2B	-2.04	1.46	1.50
25	y	308	CLA	CMC-C2C	-2.04	1.46	1.50
25	q	315	CLA	CMB-C2B	-2.04	1.46	1.50
30	A	601	LHG	O7-C7	2.04	1.40	1.34
25	B	605	CLA	CHC-C1C	2.04	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	314	CLA	CMD-C2D	-2.04	1.46	1.50
24	7	312	CHL	CHB-C4A	-2.04	1.32	1.37
32	D	409	SQD	O4-C4	-2.04	1.38	1.43
31	B	617	8CT	C33-C32	-2.04	1.44	1.50
25	u	308	CLA	CMB-C2B	-2.04	1.46	1.50
25	R	604	CLA	CHC-C1C	2.04	1.42	1.38
25	7	314	CLA	CHC-C1C	2.04	1.42	1.38
25	r	311	CLA	CMD-C2D	-2.04	1.46	1.50
25	2	316	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	608	CLA	CHC-C1C	2.04	1.42	1.38
39	D	406	PL9	C7-C8	-2.04	1.47	1.50
25	6	306	CLA	CMB-C2B	-2.04	1.46	1.50
25	7	316	CLA	CHC-C1C	2.04	1.42	1.38
25	B	609	CLA	CMC-C2C	-2.04	1.46	1.50
25	s	410	CLA	CMC-C2C	-2.04	1.46	1.50
24	u	318	CHL	C2C-C1C	2.04	1.48	1.44
25	8	306	CLA	CHC-C1C	2.04	1.42	1.38
25	B	605	CLA	CMC-C2C	-2.04	1.46	1.50
25	6	315	CLA	CMC-C2C	-2.04	1.46	1.50
32	B	618	SQD	O4-C4	-2.04	1.38	1.43
24	9	305	CHL	CHB-C4A	-2.04	1.32	1.37
25	u	308	CLA	CMD-C2D	-2.04	1.46	1.50
25	p	307	CLA	CHC-C1C	2.04	1.42	1.38
24	n	311	CHL	C4C-C3C	2.04	1.48	1.45
25	4	314	CLA	CMD-C2D	-2.04	1.46	1.50
24	N	311	CHL	C2C-C1C	2.04	1.48	1.44
25	8	312	CLA	CHC-C1C	2.04	1.42	1.38
24	S	601	CHL	C4C-C3C	2.04	1.48	1.45
25	6	316	CLA	CMB-C2B	-2.04	1.46	1.50
25	p	315	CLA	CMC-C2C	-2.04	1.46	1.50
24	1	305	CHL	CHB-C4A	-2.04	1.32	1.37
25	C	611	CLA	CHC-C1C	2.04	1.42	1.38
25	2	314	CLA	CMD-C2D	-2.04	1.46	1.50
25	p	317	CLA	CMC-C2C	-2.04	1.46	1.50
30	d	407	LHG	O7-C7	2.04	1.40	1.34
24	Y	312	CHL	C4C-C3C	2.03	1.48	1.45
24	p	313	CHL	CHB-C4A	-2.03	1.32	1.37
24	7	313	CHL	CHB-C4A	-2.03	1.32	1.37
25	2	316	CLA	CHC-C1C	2.03	1.42	1.38
24	3	311	CHL	C2C-C1C	2.03	1.48	1.44
25	R	604	CLA	CMC-C2C	-2.03	1.46	1.50
25	9	316	CLA	CMC-C2C	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	314	CLA	CMD-C2D	-2.03	1.46	1.50
25	s	417	CLA	CHC-C1C	2.03	1.42	1.38
25	8	313	CLA	CMC-C2C	-2.03	1.46	1.50
25	a	603	CLA	MG-ND	-2.03	2.01	2.05
25	r	305	CLA	CHC-C1C	2.03	1.42	1.38
25	u	317	CLA	CMC-C2C	-2.03	1.46	1.50
25	q	305	CLA	CMC-C2C	-2.03	1.46	1.50
32	b	618	SQD	O3-C3	-2.03	1.38	1.43
25	R	610	CLA	CMD-C2D	-2.03	1.46	1.50
25	9	315	CLA	CMD-C2D	-2.03	1.46	1.50
25	N	316	CLA	CMB-C2B	-2.03	1.46	1.50
25	g	316	CLA	CMC-C2C	-2.03	1.46	1.50
25	n	306	CLA	CMD-C2D	-2.03	1.46	1.50
25	8	313	CLA	CMB-C2B	-2.03	1.46	1.50
25	6	316	CLA	CMD-C2D	-2.03	1.46	1.50
25	q	312	CLA	CMC-C2C	-2.03	1.46	1.50
30	a	601	LHG	O7-C7	2.03	1.40	1.34
39	D	406	PL9	C41-C39	-2.03	1.47	1.51
25	C	605	CLA	CHC-C1C	2.03	1.42	1.38
25	1	315	CLA	CMD-C2D	-2.03	1.46	1.50
25	A	603	CLA	CHC-C1C	2.03	1.42	1.38
25	a	603	CLA	CHC-C1C	2.03	1.42	1.38
25	3	315	CLA	CMB-C2B	-2.03	1.46	1.50
24	9	317	CHL	C2C-C1C	2.03	1.48	1.44
24	9	317	CHL	C1C-NC	-2.03	1.34	1.37
24	8	315	CHL	C1C-NC	-2.03	1.34	1.37
24	4	317	CHL	C1C-NC	-2.03	1.34	1.37
24	p	312	CHL	CHB-C4A	-2.03	1.32	1.37
32	b	618	SQD	O4-C4	-2.03	1.38	1.43
25	Y	315	CLA	MG-ND	-2.03	2.01	2.05
25	c	610	CLA	MG-ND	-2.03	2.01	2.05
31	B	617	8CT	C25-C26	2.03	1.38	1.35
25	B	613	CLA	CMC-C2C	-2.03	1.46	1.50
25	g	314	CLA	CMD-C2D	-2.03	1.46	1.50
30	D	407	LHG	O7-C7	2.03	1.40	1.34
24	s	408	CHL	C4C-C3C	2.03	1.48	1.45
24	p	309	CHL	C2C-C1C	2.03	1.48	1.44
25	1	306	CLA	CMD-C2D	-2.03	1.46	1.50
25	8	314	CLA	CMC-C2C	-2.03	1.46	1.50
25	R	610	CLA	CMC-C2C	-2.03	1.46	1.50
25	y	317	CLA	CHC-C1C	2.03	1.42	1.38
25	g	316	CLA	CMB-C2B	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	312	CHL	CHB-C4A	-2.03	1.32	1.37
31	b	617	8CT	C33-C32	-2.03	1.44	1.50
25	G	307	CLA	CMD-C2D	-2.03	1.46	1.50
25	8	314	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	601	CLA	CMC-C2C	-2.03	1.46	1.50
25	b	610	CLA	CHC-C1C	2.03	1.42	1.38
25	S	603	CLA	CMC-C2C	-2.03	1.46	1.50
24	R	606	CHL	C4C-C3C	2.03	1.48	1.45
24	3	305	CHL	CHB-C4A	-2.03	1.32	1.37
25	b	601	CLA	CMC-C2C	-2.03	1.46	1.50
24	y	311	CHL	C4C-C3C	2.03	1.48	1.45
24	n	317	CHL	C2C-C1C	2.03	1.48	1.44
25	g	317	CLA	CMC-C2C	-2.02	1.46	1.50
24	p	311	CHL	C4C-C3C	2.02	1.48	1.45
25	B	602	CLA	CMC-C2C	-2.02	1.46	1.50
25	4	307	CLA	CMD-C2D	-2.02	1.46	1.50
25	q	315	CLA	CMC-C2C	-2.02	1.46	1.50
25	s	411	CLA	CMC-C2C	-2.02	1.46	1.50
24	6	305	CHL	CHB-C4A	-2.02	1.32	1.37
25	3	316	CLA	CMB-C2B	-2.02	1.46	1.50
25	7	315	CLA	CMC-C2C	-2.02	1.46	1.50
25	C	611	CLA	C1B-NB	-2.02	1.35	1.37
25	5	316	CLA	CHC-C1C	2.02	1.42	1.38
24	G	310	CHL	C2C-C1C	2.02	1.48	1.44
25	S	612	CLA	CHC-C1C	2.02	1.42	1.38
25	2	308	CLA	CMD-C2D	-2.02	1.46	1.50
25	r	305	CLA	CMC-C2C	-2.02	1.46	1.50
24	N	317	CHL	C2C-C1C	2.02	1.48	1.44
25	a	604	CLA	C1B-C2B	2.02	1.48	1.43
25	C	612	CLA	CHC-C1C	2.02	1.42	1.38
39	d	406	PL9	C41-C39	-2.02	1.47	1.51
25	R	613	CLA	CMD-C2D	-2.02	1.46	1.50
25	2	314	CLA	CMB-C2B	-2.02	1.46	1.50
25	6	306	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	602	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	612	CLA	CHC-C1C	2.02	1.42	1.38
25	8	312	CLA	CMB-C2B	-2.02	1.46	1.50
24	p	311	CHL	C2C-C1C	2.02	1.48	1.44
24	s	403	CHL	CHB-C4A	-2.02	1.32	1.37
25	g	314	CLA	CMC-C2C	-2.02	1.46	1.50
24	7	310	CHL	C2C-C1C	2.02	1.48	1.44
24	g	306	CHL	CHB-C4A	-2.02	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	CHC-C1C	2.02	1.42	1.38
25	5	308	CLA	CMD-C2D	-2.02	1.46	1.50
25	p	314	CLA	CMC-C2C	-2.02	1.46	1.50
23	f	201	HEM	CMB-C2B	2.02	1.55	1.50
24	3	317	CHL	C2C-C1C	2.02	1.48	1.44
25	C	610	CLA	CHC-C1C	2.02	1.42	1.38
25	D	404	CLA	CHC-C1C	2.02	1.42	1.38
24	2	310	CHL	C4C-C3C	2.02	1.48	1.45
25	1	313	CLA	CMD-C2D	-2.02	1.46	1.50
25	3	306	CLA	CMB-C2B	-2.02	1.46	1.50
30	n	318	LHG	P-O6	2.02	1.67	1.59
24	n	308	CHL	C2C-C1C	2.02	1.48	1.44
25	c	602	CLA	C1B-NB	-2.02	1.35	1.37
25	3	316	CLA	CMD-C2D	-2.02	1.46	1.50
25	g	307	CLA	CMD-C2D	-2.02	1.46	1.50
24	q	307	CHL	CHB-C4A	-2.02	1.32	1.37
24	2	310	CHL	CHB-C4A	-2.02	1.32	1.37
24	s	402	CHL	C4C-C3C	2.02	1.48	1.45
39	D	406	PL9	C26-C24	-2.02	1.47	1.51
25	6	315	CLA	CMB-C2B	-2.02	1.46	1.50
24	2	306	CHL	C4C-C3C	2.02	1.48	1.45
25	R	609	CLA	CHC-C1C	2.02	1.42	1.38
25	B	613	CLA	CHC-C1C	2.02	1.42	1.38
25	r	310	CLA	CHC-C1C	2.02	1.42	1.38
25	4	315	CLA	CMD-C2D	-2.01	1.46	1.50
25	9	306	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	601	CLA	CHC-C1C	2.01	1.42	1.38
24	8	309	CHL	CHB-C4A	-2.01	1.32	1.37
24	5	311	CHL	C2C-C1C	2.01	1.48	1.44
25	N	313	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	612	CLA	C1B-NB	-2.01	1.35	1.37
24	2	311	CHL	C2C-C1C	2.01	1.48	1.44
24	g	310	CHL	C2C-C1C	2.01	1.48	1.44
25	n	315	CLA	CMB-C2B	-2.01	1.46	1.50
30	N	318	LHG	P-O6	2.01	1.67	1.59
25	2	317	CLA	CHC-C1C	2.01	1.42	1.38
25	d	404	CLA	MG-ND	-2.01	2.01	2.05
25	7	314	CLA	CMC-C2C	-2.01	1.46	1.50
24	7	309	CHL	C2C-C1C	2.01	1.48	1.44
25	q	313	CLA	CHC-C1C	2.01	1.42	1.38
25	9	307	CLA	CMD-C2D	-2.01	1.46	1.50
24	1	309	CHL	C2C-C1C	2.01	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	305	CLA	CMC-C2C	-2.01	1.46	1.50
25	S	610	CLA	CHC-C1C	2.01	1.42	1.38
24	n	310	CHL	C2C-C1C	2.01	1.48	1.44
24	n	309	CHL	CHB-C4A	-2.01	1.32	1.37
25	C	607	CLA	C1B-NB	-2.01	1.35	1.37
25	c	611	CLA	C1B-NB	-2.01	1.35	1.37
25	5	316	CLA	CMB-C2B	-2.01	1.46	1.50
25	n	313	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	609	CLA	CMC-C2C	-2.01	1.46	1.50
24	4	304	CHL	C2C-C1C	2.01	1.48	1.44
24	u	310	CHL	C2C-C1C	2.01	1.48	1.44
24	6	305	CHL	C1C-NC	-2.01	1.34	1.37
25	1	307	CLA	CMD-C2D	-2.01	1.46	1.50
25	r	304	CLA	CMC-C2C	-2.01	1.46	1.50
25	D	404	CLA	MG-ND	-2.01	2.01	2.05
25	c	602	CLA	MG-ND	-2.01	2.01	2.05
35	A	606	PHO	CBD-CGD	-2.01	1.49	1.52
25	c	616	CLA	MG-ND	-2.01	2.01	2.05
24	8	307	CHL	CHB-C4A	-2.01	1.32	1.37
25	q	306	CLA	CMC-C2C	-2.01	1.46	1.50
25	b	614	CLA	MG-ND	-2.01	2.01	2.05
25	A	603	CLA	C1B-NB	-2.01	1.35	1.37
25	3	313	CLA	CMD-C2D	-2.01	1.46	1.50
25	5	317	CLA	CMB-C2B	-2.01	1.46	1.50
25	g	308	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	606	CLA	MG-ND	-2.01	2.01	2.05
39	d	406	PL9	C11-C9	-2.01	1.47	1.51
30	G	319	LHG	P-O6	2.01	1.67	1.59
25	3	307	CLA	CMD-C2D	-2.01	1.46	1.50
24	4	308	CHL	C2C-C1C	2.01	1.48	1.44
25	N	316	CLA	CMD-C2D	-2.01	1.46	1.50
25	S	609	CLA	CHC-C1C	2.01	1.42	1.38
25	c	611	CLA	CHC-C1C	2.01	1.42	1.38
25	2	317	CLA	CMB-C2B	-2.00	1.46	1.50
25	r	310	CLA	CMB-C2B	-2.00	1.46	1.50
25	A	604	CLA	C1B-C2B	2.00	1.48	1.43
24	r	306	CHL	C2C-C1C	2.00	1.48	1.44
25	q	306	CLA	CHC-C1C	2.00	1.42	1.38
24	Y	310	CHL	C4C-C3C	2.00	1.48	1.45
25	N	315	CLA	CMB-C2B	-2.00	1.46	1.50
24	y	310	CHL	C2C-C1C	2.00	1.48	1.44
25	C	603	CLA	CHC-C1C	2.00	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	310	CHL	C4C-C3C	2.00	1.48	1.45
24	S	608	CHL	CHB-C4A	-2.00	1.32	1.37
24	4	305	CHL	CHB-C4A	-2.00	1.32	1.37
25	s	411	CLA	CHC-C1C	2.00	1.42	1.38
24	R	602	CHL	C4C-C3C	2.00	1.48	1.45
25	R	612	CLA	CMB-C2B	-2.00	1.46	1.50
25	6	307	CLA	CMD-C2D	-2.00	1.46	1.50
25	1	314	CLA	CMD-C2D	-2.00	1.46	1.50
25	G	317	CLA	CMC-C2C	-2.00	1.46	1.50
25	5	315	CLA	CMC-C2C	-2.00	1.46	1.50
24	2	309	CHL	C2C-C1C	2.00	1.48	1.44
25	4	314	CLA	CMB-C2B	-2.00	1.46	1.50

All (7347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	416	8CT	C22-C21-C20	-31.40	78.94	122.92
31	S	615	8CT	C22-C21-C20	-31.38	78.96	122.92
31	S	615	8CT	C22-C21-C23	-25.32	78.18	118.08
31	s	416	8CT	C22-C21-C23	-25.31	78.20	118.08
31	S	615	8CT	C23-C21-C20	24.86	157.09	118.94
31	s	416	8CT	C23-C21-C20	24.86	157.08	118.94
28	G	304	NEX	O24-C25-C24	19.77	128.24	113.38
28	4	303	NEX	O24-C25-C24	19.72	128.20	113.38
28	u	304	NEX	O24-C25-C24	19.71	128.19	113.38
28	r	317	NEX	O24-C25-C24	19.71	128.19	113.38
28	p	304	NEX	O24-C25-C24	19.71	128.19	113.38
28	1	303	NEX	O24-C25-C24	19.70	128.18	113.38
28	5	304	NEX	O24-C25-C24	19.70	128.18	113.38
28	2	304	NEX	O24-C25-C24	19.69	128.17	113.38
28	g	304	NEX	O24-C25-C24	19.69	128.17	113.38
28	7	304	NEX	O24-C25-C24	19.69	128.17	113.38
28	S	617	NEX	O24-C25-C24	19.68	128.17	113.38
28	9	319	NEX	O24-C25-C24	19.68	128.17	113.38
28	R	616	NEX	O24-C25-C24	19.66	128.15	113.38
28	y	304	NEX	O24-C25-C24	19.66	128.15	113.38
28	S	617	NEX	C20-C13-C12	13.51	139.36	118.08
28	p	304	NEX	C20-C13-C12	13.50	139.35	118.08
28	r	317	NEX	C20-C13-C12	13.50	139.34	118.08
28	G	304	NEX	C20-C13-C12	13.50	139.34	118.08
28	4	303	NEX	C20-C13-C12	13.49	139.34	118.08
28	5	304	NEX	C20-C13-C12	13.49	139.34	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	304	NEX	C20-C13-C12	13.49	139.34	118.08
28	7	304	NEX	C20-C13-C12	13.49	139.33	118.08
28	2	304	NEX	C20-C13-C12	13.49	139.33	118.08
28	u	304	NEX	C20-C13-C12	13.49	139.33	118.08
28	y	304	NEX	C20-C13-C12	13.48	139.32	118.08
28	R	616	NEX	C20-C13-C12	13.48	139.31	118.08
28	1	303	NEX	C20-C13-C12	13.47	139.30	118.08
28	9	319	NEX	C20-C13-C12	13.46	139.28	118.08
28	y	304	NEX	C12-C13-C14	-12.17	100.26	118.94
28	G	304	NEX	C12-C13-C14	-12.17	100.27	118.94
28	2	304	NEX	C12-C13-C14	-12.16	100.27	118.94
28	4	303	NEX	C12-C13-C14	-12.16	100.28	118.94
28	S	617	NEX	C12-C13-C14	-12.16	100.28	118.94
28	p	304	NEX	C12-C13-C14	-12.16	100.29	118.94
28	5	304	NEX	C12-C13-C14	-12.15	100.29	118.94
28	r	317	NEX	C12-C13-C14	-12.15	100.29	118.94
28	9	319	NEX	C12-C13-C14	-12.15	100.30	118.94
28	7	304	NEX	C12-C13-C14	-12.14	100.31	118.94
28	g	304	NEX	C12-C13-C14	-12.13	100.33	118.94
28	u	304	NEX	C12-C13-C14	-12.13	100.33	118.94
28	R	616	NEX	C12-C13-C14	-12.12	100.34	118.94
28	1	303	NEX	C12-C13-C14	-12.12	100.35	118.94
31	S	615	8CT	C33-C32-C31	-11.23	114.08	124.85
28	N	303	NEX	O24-C25-C24	11.18	121.78	113.38
28	3	318	NEX	O24-C25-C24	11.18	121.78	113.38
31	s	416	8CT	C33-C32-C31	-11.17	114.14	124.85
28	s	401	NEX	O24-C25-C24	11.17	121.77	113.38
28	6	303	NEX	O24-C25-C24	11.17	121.77	113.38
28	r	301	NEX	O24-C25-C24	11.14	121.75	113.38
28	n	303	NEX	O24-C25-C24	11.14	121.75	113.38
31	T	101	8CT	C33-C32-C31	-10.93	114.37	124.85
31	t	101	8CT	C33-C32-C31	-10.91	114.39	124.85
24	p	306	CHL	C2B-C1B-NB	10.75	117.44	110.23
24	y	306	CHL	C2B-C1B-NB	10.70	117.41	110.23
24	Y	305	CHL	C2B-C1B-NB	10.68	117.39	110.23
24	7	306	CHL	C2B-C1B-NB	10.61	117.35	110.23
24	y	311	CHL	C2B-C1B-NB	10.54	117.30	110.23
24	Y	309	CHL	C2B-C1B-NB	10.48	117.26	110.23
24	Y	310	CHL	C2B-C1B-NB	10.46	117.25	110.23
24	y	310	CHL	C2B-C1B-NB	10.43	117.22	110.23
24	S	607	CHL	C2B-C1B-NB	10.41	117.21	110.23
24	p	312	CHL	C2B-C1B-NB	10.41	117.21	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	309	CHL	C2B-C1B-NB	10.40	117.20	110.23
24	p	305	CHL	C2B-C1B-NB	10.39	117.20	110.23
24	7	305	CHL	C2B-C1B-NB	10.37	117.19	110.23
24	7	312	CHL	C2B-C1B-NB	10.36	117.18	110.23
24	R	605	CHL	C2B-C1B-NB	10.35	117.17	110.23
24	R	607	CHL	C2B-C1B-NB	10.35	117.17	110.23
24	Y	311	CHL	C2B-C1B-NB	10.34	117.16	110.23
24	y	312	CHL	C2B-C1B-NB	10.34	117.16	110.23
24	r	308	CHL	C2B-C1B-NB	10.33	117.16	110.23
24	S	601	CHL	C2B-C1B-NB	10.33	117.16	110.23
24	s	408	CHL	C2B-C1B-NB	10.31	117.14	110.23
24	5	312	CHL	C2B-C1B-NB	10.29	117.13	110.23
24	s	402	CHL	C2B-C1B-NB	10.28	117.12	110.23
24	2	312	CHL	C2B-C1B-NB	10.28	117.12	110.23
24	1	305	CHL	C2B-C1B-NB	10.28	117.12	110.23
24	y	305	CHL	C2B-C1B-NB	10.28	117.12	110.23
24	Y	304	CHL	C2B-C1B-NB	10.28	117.12	110.23
24	4	305	CHL	C2B-C1B-NB	10.25	117.10	110.23
24	N	309	CHL	C2B-C1B-NB	10.16	117.04	110.23
24	n	311	CHL	C2B-C1B-NB	10.14	117.03	110.23
24	5	309	CHL	C4D-CHA-C1A	-10.13	108.92	121.25
24	6	311	CHL	C2B-C1B-NB	10.11	117.01	110.23
24	N	311	CHL	C2B-C1B-NB	10.10	117.00	110.23
24	q	307	CHL	C4D-CHA-C1A	-10.10	108.96	121.25
24	q	308	CHL	C2B-C1B-NB	10.08	116.99	110.23
24	y	318	CHL	C2B-C1B-NB	10.08	116.99	110.23
24	8	307	CHL	C4D-CHA-C1A	-10.06	109.00	121.25
24	R	606	CHL	C2B-C1B-NB	10.05	116.97	110.23
24	8	308	CHL	C2B-C1B-NB	10.04	116.97	110.23
24	2	309	CHL	C4D-CHA-C1A	-10.01	109.07	121.25
24	8	310	CHL	C2B-C1B-NB	10.01	116.94	110.23
24	6	308	CHL	C4D-CHA-C1A	-10.01	109.07	121.25
24	Y	317	CHL	C2B-C1B-NB	10.00	116.94	110.23
24	q	311	CHL	C2B-C1B-NB	9.99	116.93	110.23
24	y	309	CHL	C4D-CHA-C1A	-9.98	109.10	121.25
24	S	613	CHL	C2B-C1B-NB	9.97	116.92	110.23
24	g	306	CHL	C2B-C1B-NB	9.97	116.92	110.23
24	Y	308	CHL	C4D-CHA-C1A	-9.96	109.13	121.25
24	u	310	CHL	C4D-CHA-C1A	-9.95	109.14	121.25
24	2	306	CHL	C2B-C1B-NB	9.95	116.90	110.23
24	5	306	CHL	C2B-C1B-NB	9.95	116.90	110.23
24	4	308	CHL	C4D-CHA-C1A	-9.95	109.14	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	308	CHL	C4D-CHA-C1A	-9.95	109.14	121.25
24	g	318	CHL	C2B-C1B-NB	9.94	116.90	110.23
24	4	317	CHL	C4D-CHA-C1A	-9.94	109.15	121.25
24	R	602	CHL	C2B-C1B-NB	9.94	116.90	110.23
24	g	309	CHL	C4D-CHA-C1A	-9.94	109.16	121.25
24	r	308	CHL	C4D-CHA-C1A	-9.93	109.17	121.25
24	r	303	CHL	C2B-C1B-NB	9.93	116.89	110.23
24	1	317	CHL	C4D-CHA-C1A	-9.92	109.18	121.25
24	G	318	CHL	C2B-C1B-NB	9.92	116.88	110.23
24	9	309	CHL	C4D-CHA-C1A	-9.89	109.21	121.25
24	R	607	CHL	C4D-CHA-C1A	-9.89	109.22	121.25
24	5	305	CHL	C2B-C1B-NB	9.88	116.86	110.23
24	1	308	CHL	C4D-CHA-C1A	-9.88	109.22	121.25
24	G	309	CHL	C4D-CHA-C1A	-9.88	109.22	121.25
24	1	311	CHL	C2B-C1B-NB	9.88	116.86	110.23
24	G	306	CHL	C2B-C1B-NB	9.87	116.85	110.23
24	1	309	CHL	C4D-CHA-C1A	-9.87	109.24	121.25
24	s	414	CHL	C2B-C1B-NB	9.87	116.85	110.23
24	q	308	CHL	C4D-CHA-C1A	-9.87	109.24	121.25
24	r	307	CHL	C2B-C1B-NB	9.86	116.84	110.23
24	5	310	CHL	C2B-C1B-NB	9.85	116.84	110.23
24	8	308	CHL	C4D-CHA-C1A	-9.85	109.26	121.25
24	3	311	CHL	C2B-C1B-NB	9.85	116.84	110.23
24	n	317	CHL	C4D-CHA-C1A	-9.85	109.27	121.25
24	4	309	CHL	C4D-CHA-C1A	-9.84	109.27	121.25
24	9	308	CHL	C4D-CHA-C1A	-9.84	109.28	121.25
24	G	305	CHL	C2B-C1B-NB	9.84	116.83	110.23
24	u	309	CHL	C4D-CHA-C1A	-9.84	109.28	121.25
24	N	317	CHL	C4D-CHA-C1A	-9.83	109.28	121.25
24	G	310	CHL	C4D-CHA-C1A	-9.83	109.29	121.25
24	N	311	CHL	C4D-CHA-C1A	-9.82	109.29	121.25
24	g	310	CHL	C4D-CHA-C1A	-9.81	109.31	121.25
24	S	608	CHL	C2B-C1B-NB	9.80	116.81	110.23
24	8	315	CHL	C4D-CHA-C1A	-9.80	109.32	121.25
24	u	305	CHL	C4D-CHA-C1A	-9.80	109.33	121.25
24	g	305	CHL	C2B-C1B-NB	9.79	116.80	110.23
24	u	312	CHL	C4D-CHA-C1A	-9.79	109.33	121.25
24	2	305	CHL	C2B-C1B-NB	9.79	116.80	110.23
24	7	309	CHL	C4D-CHA-C1A	-9.78	109.35	121.25
24	2	310	CHL	C2B-C1B-NB	9.78	116.79	110.23
24	p	309	CHL	C4D-CHA-C1A	-9.78	109.35	121.25
24	Y	319	CHL	C2B-C1B-NB	9.77	116.78	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	u	318	CHL	C4D-CHA-C1A	-9.77	109.36	121.25
24	8	309	CHL	C2B-C1B-NB	9.77	116.78	110.23
24	2	305	CHL	C4D-CHA-C1A	-9.76	109.37	121.25
24	9	311	CHL	C4D-CHA-C1A	-9.76	109.37	121.25
24	9	317	CHL	C4D-CHA-C1A	-9.76	109.37	121.25
24	y	310	CHL	C4D-CHA-C1A	-9.76	109.38	121.25
24	q	304	CHL	C2B-C1B-NB	9.76	116.77	110.23
24	s	403	CHL	C4D-CHA-C1A	-9.76	109.38	121.25
24	p	312	CHL	C4D-CHA-C1A	-9.75	109.39	121.25
24	q	310	CHL	C2B-C1B-NB	9.75	116.77	110.23
24	Y	309	CHL	C4D-CHA-C1A	-9.74	109.39	121.25
24	n	311	CHL	C4D-CHA-C1A	-9.74	109.39	121.25
24	S	602	CHL	C4D-CHA-C1A	-9.74	109.39	121.25
24	r	303	CHL	C4D-CHA-C1A	-9.74	109.40	121.25
24	n	304	CHL	C4D-CHA-C1A	-9.73	109.41	121.25
24	G	305	CHL	C4D-CHA-C1A	-9.73	109.41	121.25
24	3	317	CHL	C4D-CHA-C1A	-9.73	109.41	121.25
24	S	606	CHL	C2B-C1B-NB	9.72	116.75	110.23
24	3	311	CHL	C4D-CHA-C1A	-9.72	109.42	121.25
24	q	316	CHL	C4D-CHA-C1A	-9.72	109.42	121.25
24	q	309	CHL	C2B-C1B-NB	9.72	116.75	110.23
24	7	318	CHL	C2B-C1B-NB	9.72	116.75	110.23
24	5	318	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
24	q	309	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
24	8	304	CHL	C2B-C1B-NB	9.71	116.74	110.23
24	4	311	CHL	C2B-C1B-NB	9.71	116.74	110.23
24	g	305	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
24	p	310	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
24	3	304	CHL	C2B-C1B-NB	9.71	116.74	110.23
24	7	310	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
24	7	312	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
24	s	407	CHL	C2B-C1B-NB	9.71	116.74	110.23
24	y	309	CHL	C2B-C1B-NB	9.70	116.74	110.23
24	p	318	CHL	C2B-C1B-NB	9.69	116.73	110.23
24	5	305	CHL	C4D-CHA-C1A	-9.69	109.45	121.25
24	Y	319	CHL	C4D-CHA-C1A	-9.69	109.46	121.25
24	N	304	CHL	C4D-CHA-C1A	-9.69	109.46	121.25
24	R	602	CHL	C4D-CHA-C1A	-9.68	109.47	121.25
24	2	318	CHL	C4D-CHA-C1A	-9.68	109.47	121.25
24	n	309	CHL	C4D-CHA-C1A	-9.68	109.47	121.25
24	Y	310	CHL	C4D-CHA-C1A	-9.68	109.47	121.25
24	9	304	CHL	C4D-CHA-C1A	-9.68	109.47	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	311	CHL	C4D-CHA-C1A	-9.68	109.47	121.25
24	6	317	CHL	C4D-CHA-C1A	-9.67	109.47	121.25
24	Y	308	CHL	C2B-C1B-NB	9.67	116.72	110.23
24	8	303	CHL	C4D-CHA-C1A	-9.67	109.48	121.25
24	n	310	CHL	C4D-CHA-C1A	-9.67	109.48	121.25
24	7	318	CHL	C4D-CHA-C1A	-9.67	109.48	121.25
24	Y	304	CHL	C4D-CHA-C1A	-9.67	109.48	121.25
24	s	408	CHL	C4D-CHA-C1A	-9.67	109.48	121.25
24	2	310	CHL	C4D-CHA-C1A	-9.66	109.49	121.25
24	q	303	CHL	C4D-CHA-C1A	-9.66	109.49	121.25
24	S	602	CHL	C2B-C1B-NB	9.66	116.71	110.23
24	N	310	CHL	C4D-CHA-C1A	-9.66	109.49	121.25
24	S	607	CHL	C4D-CHA-C1A	-9.66	109.50	121.25
24	2	312	CHL	C4D-CHA-C1A	-9.66	109.50	121.25
24	2	311	CHL	C4D-CHA-C1A	-9.65	109.50	121.25
24	5	310	CHL	C4D-CHA-C1A	-9.65	109.51	121.25
24	G	318	CHL	C4D-CHA-C1A	-9.64	109.51	121.25
24	s	409	CHL	C2B-C1B-NB	9.64	116.69	110.23
24	4	305	CHL	C4D-CHA-C1A	-9.64	109.52	121.25
24	p	318	CHL	C4D-CHA-C1A	-9.64	109.52	121.25
24	N	309	CHL	C4D-CHA-C1A	-9.64	109.52	121.25
24	g	318	CHL	C4D-CHA-C1A	-9.63	109.53	121.25
24	6	310	CHL	C4D-CHA-C1A	-9.63	109.53	121.25
24	y	311	CHL	C4D-CHA-C1A	-9.63	109.53	121.25
24	y	305	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
24	s	406	CHL	C2B-C1B-NB	9.62	116.68	110.23
24	5	312	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
24	4	310	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
24	1	305	CHL	C4D-CHA-C1A	-9.61	109.55	121.25
24	3	310	CHL	C4D-CHA-C1A	-9.61	109.56	121.25
24	5	311	CHL	C4D-CHA-C1A	-9.60	109.57	121.25
24	8	307	CHL	C2B-C1B-NB	9.60	116.67	110.23
24	S	605	CHL	C2B-C1B-NB	9.59	116.66	110.23
24	Y	312	CHL	C4D-CHA-C1A	-9.59	109.58	121.25
24	5	313	CHL	C4D-CHA-C1A	-9.58	109.59	121.25
24	g	306	CHL	C4D-CHA-C1A	-9.58	109.59	121.25
24	Y	312	CHL	C2B-C1B-NB	9.57	116.65	110.23
24	4	310	CHL	C2B-C1B-NB	9.57	116.65	110.23
24	q	310	CHL	C4D-CHA-C1A	-9.57	109.61	121.25
24	y	313	CHL	C4D-CHA-C1A	-9.57	109.61	121.25
24	1	310	CHL	C4D-CHA-C1A	-9.57	109.61	121.25
24	r	306	CHL	C4D-CHA-C1A	-9.56	109.61	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	CHL	C4D-CHA-C1A	-9.56	109.61	121.25
24	4	311	CHL	C4D-CHA-C1A	-9.56	109.61	121.25
24	9	310	CHL	C4D-CHA-C1A	-9.55	109.62	121.25
24	2	313	CHL	C4D-CHA-C1A	-9.55	109.63	121.25
24	g	312	CHL	C2B-C1B-NB	9.55	116.63	110.23
24	1	304	CHL	C4D-CHA-C1A	-9.55	109.63	121.25
24	G	306	CHL	C4D-CHA-C1A	-9.55	109.63	121.25
24	s	403	CHL	C2B-C1B-NB	9.54	116.63	110.23
24	p	305	CHL	C4D-CHA-C1A	-9.54	109.64	121.25
24	7	305	CHL	C4D-CHA-C1A	-9.54	109.64	121.25
24	Y	317	CHL	C4D-CHA-C1A	-9.54	109.64	121.25
24	u	306	CHL	C2B-C1B-NB	9.53	116.62	110.23
24	p	313	CHL	C2B-C1B-NB	9.53	116.62	110.23
24	6	305	CHL	C4D-CHA-C1A	-9.53	109.66	121.25
24	Y	311	CHL	C4D-CHA-C1A	-9.52	109.66	121.25
24	3	305	CHL	C4D-CHA-C1A	-9.52	109.66	121.25
24	4	304	CHL	C4D-CHA-C1A	-9.52	109.66	121.25
24	8	309	CHL	C4D-CHA-C1A	-9.52	109.67	121.25
24	N	312	CHL	C2B-C1B-NB	9.52	116.61	110.23
24	u	311	CHL	C4D-CHA-C1A	-9.52	109.67	121.25
24	7	313	CHL	C2B-C1B-NB	9.51	116.61	110.23
24	r	306	CHL	C2B-C1B-NB	9.50	116.60	110.23
24	R	601	CHL	C2B-C1B-NB	9.50	116.60	110.23
24	r	302	CHL	C4D-CHA-C1A	-9.50	109.69	121.25
24	N	308	CHL	C4D-CHA-C1A	-9.50	109.69	121.25
24	R	608	CHL	C4D-CHA-C1A	-9.50	109.69	121.25
24	1	310	CHL	C2B-C1B-NB	9.50	116.60	110.23
24	n	308	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
24	R	608	CHL	C2B-C1B-NB	9.49	116.59	110.23
24	R	605	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
24	6	304	CHL	C2B-C1B-NB	9.49	116.59	110.23
24	y	318	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
24	9	304	CHL	C2B-C1B-NB	9.49	116.59	110.23
24	R	606	CHL	C4D-CHA-C1A	-9.48	109.71	121.25
24	7	311	CHL	C2B-C1B-NB	9.48	116.59	110.23
24	y	312	CHL	C4D-CHA-C1A	-9.48	109.71	121.25
24	g	313	CHL	C4D-CHA-C1A	-9.48	109.71	121.25
24	G	312	CHL	C4D-CHA-C1A	-9.48	109.71	121.25
24	r	309	CHL	C4D-CHA-C1A	-9.48	109.71	121.25
24	R	601	CHL	C4D-CHA-C1A	-9.47	109.73	121.25
24	q	307	CHL	C2B-C1B-NB	9.47	116.58	110.23
24	r	309	CHL	C2B-C1B-NB	9.46	116.58	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	304	CHL	C4D-CHA-C1A	-9.46	109.74	121.25
24	r	302	CHL	C2B-C1B-NB	9.46	116.57	110.23
24	9	305	CHL	C2B-C1B-NB	9.45	116.57	110.23
24	G	311	CHL	C2B-C1B-NB	9.45	116.57	110.23
24	9	305	CHL	C4D-CHA-C1A	-9.44	109.75	121.25
24	p	311	CHL	C2B-C1B-NB	9.44	116.56	110.23
24	n	312	CHL	C2B-C1B-NB	9.44	116.56	110.23
24	6	304	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
24	S	605	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
24	9	312	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
24	S	613	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
24	N	305	CHL	C2B-C1B-NB	9.43	116.56	110.23
24	8	304	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
24	u	312	CHL	C2B-C1B-NB	9.43	116.55	110.23
24	g	312	CHL	C4D-CHA-C1A	-9.43	109.78	121.25
24	N	304	CHL	C2B-C1B-NB	9.43	116.55	110.23
24	S	601	CHL	C4D-CHA-C1A	-9.42	109.78	121.25
24	p	311	CHL	C4D-CHA-C1A	-9.42	109.79	121.25
24	s	409	CHL	C4D-CHA-C1A	-9.42	109.79	121.25
24	9	311	CHL	C2B-C1B-NB	9.41	116.54	110.23
24	u	306	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
24	3	304	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
24	r	307	CHL	C4D-CHA-C1A	-9.40	109.80	121.25
24	G	313	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
24	s	406	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
24	s	402	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
24	S	608	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
24	3	309	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
24	n	305	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
24	s	414	CHL	C4D-CHA-C1A	-9.39	109.82	121.25
24	G	312	CHL	C2B-C1B-NB	9.39	116.53	110.23
24	1	312	CHL	C4D-CHA-C1A	-9.39	109.82	121.25
31	S	614	8CT	C33-C32-C31	-9.39	115.85	124.85
24	6	309	CHL	C4D-CHA-C1A	-9.37	109.84	121.25
24	6	312	CHL	C4D-CHA-C1A	-9.37	109.84	121.25
24	G	311	CHL	C4D-CHA-C1A	-9.36	109.85	121.25
24	7	311	CHL	C4D-CHA-C1A	-9.36	109.86	121.25
24	3	312	CHL	C4D-CHA-C1A	-9.36	109.86	121.25
24	N	305	CHL	C4D-CHA-C1A	-9.36	109.86	121.25
24	N	308	CHL	C2B-C1B-NB	9.35	116.50	110.23
24	n	310	CHL	C2B-C1B-NB	9.35	116.50	110.23
24	u	305	CHL	C2B-C1B-NB	9.35	116.50	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	310	CHL	C2B-C1B-NB	9.34	116.50	110.23
24	6	305	CHL	C2B-C1B-NB	9.34	116.49	110.23
24	S	606	CHL	C4D-CHA-C1A	-9.34	109.89	121.25
24	u	313	CHL	C4D-CHA-C1A	-9.34	109.89	121.25
24	p	306	CHL	C4D-CHA-C1A	-9.33	109.89	121.25
24	q	311	CHL	C4D-CHA-C1A	-9.33	109.90	121.25
24	7	313	CHL	C4D-CHA-C1A	-9.33	109.90	121.25
31	s	415	8CT	C33-C32-C31	-9.32	115.91	124.85
31	c	615	8CT	C33-C32-C31	-9.32	115.91	124.85
24	7	310	CHL	C2B-C1B-NB	9.32	116.48	110.23
24	g	311	CHL	C2B-C1B-NB	9.31	116.47	110.23
24	n	304	CHL	C2B-C1B-NB	9.31	116.47	110.23
24	2	306	CHL	C4D-CHA-C1A	-9.31	109.92	121.25
24	7	306	CHL	C4D-CHA-C1A	-9.31	109.92	121.25
24	s	407	CHL	C4D-CHA-C1A	-9.31	109.92	121.25
24	4	312	CHL	C4D-CHA-C1A	-9.31	109.92	121.25
24	y	313	CHL	C2B-C1B-NB	9.31	116.47	110.23
24	n	312	CHL	C4D-CHA-C1A	-9.31	109.92	121.25
24	g	311	CHL	C4D-CHA-C1A	-9.30	109.93	121.25
31	C	615	8CT	C33-C32-C31	-9.30	115.94	124.85
24	n	305	CHL	C2B-C1B-NB	9.30	116.46	110.23
24	p	313	CHL	C4D-CHA-C1A	-9.28	109.95	121.25
24	8	310	CHL	C4D-CHA-C1A	-9.28	109.95	121.25
24	3	305	CHL	C2B-C1B-NB	9.27	116.45	110.23
24	3	317	CHL	C2B-C1B-NB	9.26	116.44	110.23
24	u	311	CHL	C2B-C1B-NB	9.26	116.44	110.23
24	5	306	CHL	C4D-CHA-C1A	-9.26	109.98	121.25
28	5	304	NEX	C30-C31-C32	-9.25	94.35	123.22
24	N	312	CHL	C4D-CHA-C1A	-9.25	110.00	121.25
28	R	616	NEX	C30-C31-C32	-9.24	94.37	123.22
28	r	317	NEX	C30-C31-C32	-9.24	94.37	123.22
28	S	617	NEX	C30-C31-C32	-9.24	94.37	123.22
28	u	304	NEX	C30-C31-C32	-9.24	94.38	123.22
28	p	304	NEX	C30-C31-C32	-9.24	94.38	123.22
24	N	310	CHL	C2B-C1B-NB	9.24	116.43	110.23
28	7	304	NEX	C30-C31-C32	-9.24	94.39	123.22
28	G	304	NEX	C30-C31-C32	-9.23	94.40	123.22
28	9	319	NEX	C30-C31-C32	-9.23	94.40	123.22
28	y	304	NEX	C30-C31-C32	-9.23	94.41	123.22
28	g	304	NEX	C30-C31-C32	-9.23	94.41	123.22
24	6	317	CHL	C2B-C1B-NB	9.23	116.42	110.23
28	1	303	NEX	C30-C31-C32	-9.23	94.42	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	304	NEX	C30-C31-C32	-9.22	94.43	123.22
28	4	303	NEX	C30-C31-C32	-9.22	94.44	123.22
24	y	306	CHL	C4D-CHA-C1A	-9.18	110.08	121.25
24	Y	305	CHL	C4D-CHA-C1A	-9.17	110.09	121.25
24	6	309	CHL	C2B-C1B-NB	9.15	116.36	110.23
24	n	308	CHL	C2B-C1B-NB	9.14	116.36	110.23
24	2	309	CHL	C2B-C1B-NB	9.13	116.36	110.23
24	2	313	CHL	C2B-C1B-NB	9.13	116.35	110.23
24	9	310	CHL	C2B-C1B-NB	9.11	116.34	110.23
24	2	318	CHL	C2B-C1B-NB	9.10	116.33	110.23
24	9	309	CHL	C2B-C1B-NB	9.10	116.33	110.23
24	6	308	CHL	C2B-C1B-NB	9.09	116.32	110.23
24	5	313	CHL	C2B-C1B-NB	9.07	116.31	110.23
31	a	608	8CT	C33-C32-C31	-9.06	116.16	124.85
24	1	312	CHL	C2B-C1B-NB	9.06	116.31	110.23
24	5	309	CHL	C2B-C1B-NB	9.06	116.30	110.23
24	g	310	CHL	C2B-C1B-NB	9.05	116.30	110.23
24	q	303	CHL	C2B-C1B-NB	9.05	116.30	110.23
24	1	308	CHL	C2B-C1B-NB	9.05	116.30	110.23
24	3	308	CHL	C2B-C1B-NB	9.04	116.29	110.23
24	3	309	CHL	C2B-C1B-NB	9.03	116.28	110.23
31	A	608	8CT	C33-C32-C31	-9.02	116.20	124.85
24	G	310	CHL	C2B-C1B-NB	9.01	116.27	110.23
24	5	318	CHL	C2B-C1B-NB	9.01	116.27	110.23
24	u	310	CHL	C2B-C1B-NB	9.00	116.27	110.23
24	8	315	CHL	C2B-C1B-NB	9.00	116.26	110.23
24	4	312	CHL	C2B-C1B-NB	8.99	116.26	110.23
24	9	317	CHL	C2B-C1B-NB	8.99	116.26	110.23
24	4	308	CHL	C2B-C1B-NB	8.98	116.25	110.23
24	4	309	CHL	C2B-C1B-NB	8.98	116.25	110.23
24	3	310	CHL	C2B-C1B-NB	8.97	116.25	110.23
24	u	318	CHL	C2B-C1B-NB	8.96	116.24	110.23
24	q	316	CHL	C2B-C1B-NB	8.96	116.24	110.23
24	3	312	CHL	C2B-C1B-NB	8.95	116.23	110.23
24	2	311	CHL	C2B-C1B-NB	8.92	116.21	110.23
24	4	317	CHL	C2B-C1B-NB	8.89	116.19	110.23
24	u	309	CHL	C2B-C1B-NB	8.89	116.19	110.23
24	6	312	CHL	C2B-C1B-NB	8.88	116.19	110.23
24	n	317	CHL	C2B-C1B-NB	8.88	116.19	110.23
24	8	303	CHL	C2B-C1B-NB	8.86	116.17	110.23
24	N	317	CHL	C2B-C1B-NB	8.84	116.16	110.23
24	1	309	CHL	C2B-C1B-NB	8.83	116.15	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	308	CHL	C2B-C1B-NB	8.82	116.15	110.23
24	p	309	CHL	C2B-C1B-NB	8.81	116.14	110.23
24	6	310	CHL	C2B-C1B-NB	8.81	116.14	110.23
24	5	311	CHL	C2B-C1B-NB	8.81	116.14	110.23
24	1	317	CHL	C2B-C1B-NB	8.81	116.14	110.23
24	u	313	CHL	C2B-C1B-NB	8.80	116.13	110.23
31	B	617	8CT	C33-C32-C31	-8.79	116.42	124.85
24	g	313	CHL	C2B-C1B-NB	8.77	116.11	110.23
24	7	309	CHL	C2B-C1B-NB	8.76	116.10	110.23
24	G	313	CHL	C2B-C1B-NB	8.75	116.10	110.23
24	1	304	CHL	C2B-C1B-NB	8.72	116.08	110.23
24	G	309	CHL	C2B-C1B-NB	8.71	116.07	110.23
24	g	309	CHL	C2B-C1B-NB	8.71	116.07	110.23
24	9	312	CHL	C2B-C1B-NB	8.70	116.07	110.23
24	4	304	CHL	C2B-C1B-NB	8.68	116.05	110.23
31	c	614	8CT	C33-C32-C31	-8.66	116.54	124.85
28	3	318	NEX	C38-C25-C26	-8.65	107.77	122.26
28	N	303	NEX	C38-C25-C26	-8.65	107.77	122.26
28	r	301	NEX	C38-C25-C26	-8.64	107.77	122.26
28	6	303	NEX	C38-C25-C26	-8.64	107.78	122.26
28	n	303	NEX	C38-C25-C26	-8.63	107.80	122.26
28	s	401	NEX	C38-C25-C26	-8.63	107.80	122.26
31	C	614	8CT	C33-C32-C31	-8.51	116.69	124.85
31	V	401	8CT	C33-C32-C31	-8.35	116.85	124.85
31	v	401	8CT	C33-C32-C31	-8.32	116.87	124.85
31	b	617	8CT	C33-C32-C31	-8.31	116.88	124.85
31	D	410	8CT	C33-C32-C31	-8.23	116.96	124.85
31	d	410	8CT	C33-C32-C31	-8.19	117.00	124.85
27	R	615	XAT	O4-C5-C4	8.07	119.44	113.38
31	C	613	8CT	C33-C32-C31	-8.02	117.16	124.85
31	c	613	8CT	C33-C32-C31	-7.81	117.36	124.85
27	r	316	XAT	O4-C5-C4	7.74	119.19	113.38
31	X	601	8CT	C33-C32-C31	-7.63	117.53	124.85
31	B	617	8CT	C14-C13-C12	-7.62	116.43	127.31
31	x	601	8CT	C33-C32-C31	-7.54	117.62	124.85
31	b	617	8CT	C14-C13-C12	-7.52	116.58	127.31
24	s	402	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
24	R	607	CHL	CMD-C2D-C1D	7.29	137.56	124.71
25	C	611	CLA	C4A-NA-C1A	7.28	109.98	106.71
31	c	615	8CT	C24-C25-C26	-7.26	116.95	127.31
25	b	616	CLA	C4A-NA-C1A	7.26	109.97	106.71
25	B	604	CLA	C4A-NA-C1A	7.25	109.97	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	308	CHL	CMD-C2D-C1D	7.25	137.49	124.71
25	B	616	CLA	C4A-NA-C1A	7.24	109.96	106.71
25	p	315	CLA	C4A-NA-C1A	7.23	109.96	106.71
25	Y	315	CLA	C4A-NA-C1A	7.22	109.95	106.71
31	C	615	8CT	C24-C25-C26	-7.22	117.01	127.31
25	b	604	CLA	C4A-NA-C1A	7.19	109.94	106.71
25	y	316	CLA	C4A-NA-C1A	7.19	109.94	106.71
24	S	601	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
31	s	416	8CT	C04-C03-C02	-7.17	112.52	122.61
25	c	611	CLA	C4A-NA-C1A	7.15	109.92	106.71
24	3	311	CHL	CMD-C2D-C1D	7.14	137.30	124.71
28	u	304	NEX	C27-C28-C29	7.12	136.57	125.53
27	r	316	XAT	C38-C25-C26	-7.11	110.34	122.26
27	R	615	XAT	C38-C25-C26	-7.11	110.35	122.26
28	p	304	NEX	C27-C28-C29	7.10	136.55	125.53
28	2	304	NEX	C27-C28-C29	7.10	136.55	125.53
28	5	304	NEX	C27-C28-C29	7.10	136.54	125.53
28	G	304	NEX	C27-C28-C29	7.10	136.54	125.53
31	S	615	8CT	C04-C03-C02	-7.08	112.64	122.61
24	5	306	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
28	9	319	NEX	C27-C28-C29	7.08	136.51	125.53
28	4	303	NEX	C27-C28-C29	7.08	136.51	125.53
28	R	616	NEX	C27-C28-C29	7.07	136.51	125.53
28	r	317	NEX	C27-C28-C29	7.06	136.49	125.53
28	S	617	NEX	C27-C28-C29	7.06	136.49	125.53
28	7	304	NEX	C27-C28-C29	7.06	136.49	125.53
28	g	304	NEX	C27-C28-C29	7.06	136.48	125.53
28	1	303	NEX	C27-C28-C29	7.06	136.48	125.53
28	y	304	NEX	C27-C28-C29	7.06	136.48	125.53
24	6	311	CHL	CMD-C2D-C1D	7.06	137.15	124.71
24	s	403	CHL	C2C-C3C-C4C	-7.05	101.46	106.49
24	S	602	CHL	C2C-C3C-C4C	-7.05	101.46	106.49
25	c	601	CLA	C4A-NA-C1A	7.05	109.88	106.71
25	7	315	CLA	C4A-NA-C1A	7.05	109.88	106.71
24	7	306	CHL	C2C-C3C-C4C	-7.04	101.47	106.49
25	p	317	CLA	C4A-NA-C1A	7.04	109.87	106.71
25	c	607	CLA	C4A-NA-C1A	7.03	109.87	106.71
25	c	604	CLA	C4A-NA-C1A	7.01	109.86	106.71
24	Y	305	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
25	C	607	CLA	C4A-NA-C1A	7.00	109.86	106.71
24	Y	310	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
25	c	602	CLA	C4A-NA-C1A	7.00	109.85	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	306	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
25	C	612	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	p	306	CHL	C2C-C3C-C4C	-6.99	101.51	106.49
25	g	316	CLA	C4A-NA-C1A	6.97	109.84	106.71
25	b	606	CLA	C4A-NA-C1A	6.96	109.84	106.71
24	u	313	CHL	CMD-C2D-C1D	6.96	136.97	124.71
24	7	312	CHL	C2C-C3C-C4C	-6.95	101.53	106.49
24	p	305	CHL	CMD-C2D-C1D	6.95	136.96	124.71
28	y	304	NEX	C35-C34-C33	-6.95	117.40	127.31
28	G	304	NEX	C35-C34-C33	-6.95	117.40	127.31
25	B	606	CLA	C4A-NA-C1A	6.94	109.83	106.71
25	a	603	CLA	C4A-NA-C1A	6.94	109.83	106.71
28	u	304	NEX	C35-C34-C33	-6.94	117.40	127.31
24	9	305	CHL	C2C-C3C-C4C	-6.94	101.54	106.49
25	5	316	CLA	C4A-NA-C1A	6.94	109.83	106.71
24	y	311	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
28	r	317	NEX	C35-C34-C33	-6.93	117.42	127.31
28	1	303	NEX	C35-C34-C33	-6.93	117.42	127.31
24	s	408	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
25	C	602	CLA	C4A-NA-C1A	6.92	109.82	106.71
28	9	319	NEX	C35-C34-C33	-6.92	117.43	127.31
25	p	316	CLA	C4A-NA-C1A	6.92	109.82	106.71
25	b	611	CLA	C4A-NA-C1A	6.92	109.81	106.71
28	4	303	NEX	C35-C34-C33	-6.91	117.44	127.31
28	7	304	NEX	C35-C34-C33	-6.91	117.45	127.31
28	R	616	NEX	C35-C34-C33	-6.91	117.45	127.31
28	p	304	NEX	C35-C34-C33	-6.91	117.45	127.31
28	S	617	NEX	C35-C34-C33	-6.90	117.46	127.31
24	n	317	CHL	CMD-C2D-C1D	6.89	136.86	124.71
28	g	304	NEX	C35-C34-C33	-6.89	117.47	127.31
24	u	305	CHL	CMD-C2D-C1D	6.89	136.85	124.71
28	2	304	NEX	C35-C34-C33	-6.89	117.48	127.31
24	y	306	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
24	S	601	CHL	CMD-C2D-C1D	6.88	136.85	124.71
25	c	612	CLA	C4A-NA-C1A	6.88	109.80	106.71
24	N	317	CHL	CMD-C2D-C1D	6.88	136.84	124.71
24	4	311	CHL	CMD-C2D-C1D	6.88	136.84	124.71
28	5	304	NEX	C35-C34-C33	-6.88	117.49	127.31
25	A	603	CLA	C4A-NA-C1A	6.88	109.80	106.71
24	9	311	CHL	CMD-C2D-C1D	6.88	136.84	124.71
24	7	305	CHL	CMD-C2D-C1D	6.88	136.84	124.71
24	u	318	CHL	CMD-C2D-C1D	6.88	136.83	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	609	CLA	C4A-NA-C1A	6.88	109.80	106.71
25	q	314	CLA	C4A-NA-C1A	6.88	109.80	106.71
25	B	611	CLA	C4A-NA-C1A	6.87	109.80	106.71
25	C	604	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	9	317	CHL	CMD-C2D-C1D	6.87	136.83	124.71
24	g	313	CHL	CMD-C2D-C1D	6.87	136.81	124.71
24	u	312	CHL	CMD-C2D-C1D	6.86	136.81	124.71
25	r	313	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	1	311	CHL	CMD-C2D-C1D	6.86	136.80	124.71
31	x	601	8CT	C14-C13-C12	-6.86	117.52	127.31
24	y	310	CHL	C2C-C3C-C4C	-6.86	101.60	106.49
24	s	408	CHL	CMD-C2D-C1D	6.86	136.80	124.71
24	n	311	CHL	CMD-C2D-C1D	6.86	136.79	124.71
25	2	316	CLA	C4A-NA-C1A	6.85	109.79	106.71
24	N	311	CHL	CMD-C2D-C1D	6.85	136.79	124.71
24	N	309	CHL	CMD-C2D-C1D	6.85	136.79	124.71
24	s	402	CHL	CMD-C2D-C1D	6.85	136.79	124.71
25	u	315	CLA	C4A-NA-C1A	6.85	109.78	106.71
25	7	307	CLA	C4A-NA-C1A	6.85	109.78	106.71
28	9	319	NEX	C35-C15-C14	6.85	137.50	123.47
25	8	313	CLA	C4A-NA-C1A	6.84	109.78	106.71
28	p	304	NEX	C35-C15-C14	6.83	137.47	123.47
25	s	412	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	7	317	CLA	C4A-NA-C1A	6.83	109.78	106.71
24	Y	309	CHL	C2C-C3C-C4C	-6.83	101.62	106.49
24	u	306	CHL	C2C-C3C-C4C	-6.83	101.62	106.49
31	t	101	8CT	C30-C31-C32	-6.83	113.07	121.47
24	3	317	CHL	CMD-C2D-C1D	6.83	136.74	124.71
24	N	309	CHL	C2C-C3C-C4C	-6.83	101.62	106.49
24	9	304	CHL	CMD-C2D-C1D	6.83	136.74	124.71
28	5	304	NEX	C35-C15-C14	6.83	137.46	123.47
28	r	317	NEX	C35-C15-C14	6.82	137.45	123.47
28	S	617	NEX	C35-C15-C14	6.82	137.45	123.47
28	u	304	NEX	C35-C15-C14	6.82	137.45	123.47
25	r	304	CLA	C4A-NA-C1A	6.82	109.77	106.71
28	1	303	NEX	C35-C15-C14	6.82	137.45	123.47
28	g	304	NEX	C35-C15-C14	6.82	137.45	123.47
24	n	305	CHL	C2C-C3C-C4C	-6.82	101.63	106.49
31	T	101	8CT	C30-C31-C32	-6.82	113.08	121.47
28	2	304	NEX	C35-C15-C14	6.82	137.44	123.47
24	n	309	CHL	CMD-C2D-C1D	6.82	136.73	124.71
25	d	405	CLA	C4A-NA-C1A	6.82	109.77	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	316	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	5	312	CHL	CMD-C2D-C1D	6.81	136.72	124.71
24	p	312	CHL	CMD-C2D-C1D	6.81	136.72	124.71
24	7	312	CHL	CMD-C2D-C1D	6.81	136.72	124.71
24	y	310	CHL	CMD-C2D-C1D	6.81	136.72	124.71
24	y	312	CHL	C2C-C3C-C4C	-6.81	101.64	106.49
25	G	316	CLA	C4A-NA-C1A	6.81	109.77	106.71
24	S	607	CHL	C2C-C3C-C4C	-6.81	101.64	106.49
31	X	601	8CT	C14-C13-C12	-6.81	117.60	127.31
25	5	315	CLA	C4A-NA-C1A	6.80	109.77	106.71
25	b	605	CLA	C4A-NA-C1A	6.80	109.77	106.71
24	R	607	CHL	C2C-C3C-C4C	-6.80	101.64	106.49
24	q	308	CHL	CMD-C2D-C1D	6.80	136.70	124.71
28	R	616	NEX	C35-C15-C14	6.80	137.41	123.47
25	6	315	CLA	C4A-NA-C1A	6.80	109.76	106.71
24	Y	311	CHL	C2C-C3C-C4C	-6.80	101.64	106.49
24	r	303	CHL	C2C-C3C-C4C	-6.79	101.65	106.49
24	R	605	CHL	CMD-C2D-C1D	6.79	136.69	124.71
25	2	315	CLA	C4A-NA-C1A	6.79	109.76	106.71
25	p	307	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	4	317	CHL	CMD-C2D-C1D	6.79	136.68	124.71
28	7	304	NEX	C35-C15-C14	6.79	137.39	123.47
24	Y	319	CHL	CMD-C2D-C1D	6.79	136.68	124.71
24	1	305	CHL	C2C-C3C-C4C	-6.79	101.65	106.49
24	1	309	CHL	CMD-C2D-C1D	6.79	136.68	124.71
28	y	304	NEX	C35-C15-C14	6.79	137.38	123.47
25	D	405	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	4	309	CHL	CMD-C2D-C1D	6.79	136.68	124.71
25	9	314	CLA	C4A-NA-C1A	6.79	109.76	106.71
25	b	607	CLA	C4A-NA-C1A	6.79	109.76	106.71
28	G	304	NEX	C35-C15-C14	6.78	137.37	123.47
24	2	312	CHL	CMD-C2D-C1D	6.78	136.67	124.71
28	4	303	NEX	C35-C15-C14	6.78	137.37	123.47
24	6	317	CHL	CMD-C2D-C1D	6.78	136.66	124.71
24	g	309	CHL	CMD-C2D-C1D	6.78	136.66	124.71
24	S	607	CHL	CMD-C2D-C1D	6.77	136.65	124.71
24	q	308	CHL	C2C-C3C-C4C	-6.77	101.66	106.49
25	4	315	CLA	C4A-NA-C1A	6.77	109.75	106.71
24	1	317	CHL	CMD-C2D-C1D	6.77	136.64	124.71
24	8	309	CHL	CMD-C2D-C1D	6.77	136.64	124.71
24	8	308	CHL	CMD-C2D-C1D	6.77	136.64	124.71
25	C	601	CLA	C4A-NA-C1A	6.76	109.75	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	312	CHL	CMD-C2D-C1D	6.76	136.63	124.71
24	8	315	CHL	CMD-C2D-C1D	6.76	136.63	124.71
24	y	309	CHL	CMD-C2D-C1D	6.76	136.63	124.71
25	r	310	CLA	C4A-NA-C1A	6.76	109.75	106.71
24	Y	312	CHL	CMD-C2D-C1D	6.76	136.63	124.71
24	N	312	CHL	CMD-C2D-C1D	6.76	136.63	124.71
24	9	312	CHL	CMD-C2D-C1D	6.76	136.62	124.71
24	G	313	CHL	CMD-C2D-C1D	6.76	136.62	124.71
24	Y	309	CHL	CMD-C2D-C1D	6.76	136.62	124.71
25	R	603	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	B	607	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	6	304	CHL	CMD-C2D-C1D	6.75	136.61	124.71
24	Y	304	CHL	CMD-C2D-C1D	6.75	136.61	124.71
24	5	305	CHL	CMD-C2D-C1D	6.75	136.61	124.71
25	B	609	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	3	311	CHL	C2C-C3C-C4C	-6.74	101.68	106.49
24	N	305	CHL	C2C-C3C-C4C	-6.74	101.68	106.49
24	y	305	CHL	CMD-C2D-C1D	6.74	136.60	124.71
25	3	315	CLA	C4A-NA-C1A	6.74	109.74	106.71
24	R	606	CHL	C2C-C3C-C4C	-6.74	101.68	106.49
24	R	602	CHL	C2C-C3C-C4C	-6.74	101.68	106.49
25	d	404	CLA	C4A-NA-C1A	6.74	109.74	106.71
25	a	607	CLA	C4A-NA-C1A	6.74	109.74	106.71
24	8	304	CHL	C2C-C3C-C4C	-6.74	101.69	106.49
24	6	311	CHL	C2C-C3C-C4C	-6.74	101.69	106.49
24	q	316	CHL	CMD-C2D-C1D	6.74	136.59	124.71
24	G	309	CHL	CMD-C2D-C1D	6.74	136.58	124.71
24	g	306	CHL	CMD-C2D-C1D	6.73	136.58	124.71
24	3	309	CHL	C2C-C3C-C4C	-6.73	101.69	106.49
31	A	608	8CT	C14-C13-C12	-6.73	117.70	127.31
24	2	305	CHL	CMD-C2D-C1D	6.73	136.58	124.71
24	9	308	CHL	CMD-C2D-C1D	6.73	136.58	124.71
25	R	609	CLA	C4A-NA-C1A	6.73	109.73	106.71
25	u	317	CLA	C4A-NA-C1A	6.72	109.73	106.71
24	g	310	CHL	CMD-C2D-C1D	6.72	136.56	124.71
24	r	307	CHL	C2C-C3C-C4C	-6.72	101.70	106.49
24	y	313	CHL	CMD-C2D-C1D	6.72	136.56	124.71
24	p	309	CHL	CMD-C2D-C1D	6.72	136.56	124.71
24	Y	308	CHL	CMD-C2D-C1D	6.72	136.56	124.71
24	q	310	CHL	CMD-C2D-C1D	6.72	136.56	124.71
24	5	313	CHL	CMD-C2D-C1D	6.72	136.55	124.71
25	B	601	CLA	C4A-NA-C1A	6.72	109.72	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	411	CLA	C4A-NA-C1A	6.72	109.72	106.71
24	N	308	CHL	CMD-C2D-C1D	6.71	136.55	124.71
25	n	306	CLA	C4A-NA-C1A	6.71	109.72	106.71
24	q	304	CHL	C2C-C3C-C4C	-6.71	101.70	106.49
24	G	311	CHL	CMD-C2D-C1D	6.71	136.54	124.71
24	r	308	CHL	C2C-C3C-C4C	-6.71	101.71	106.49
24	n	309	CHL	C2C-C3C-C4C	-6.71	101.71	106.49
25	1	315	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	b	601	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	2	313	CHL	CMD-C2D-C1D	6.70	136.53	124.71
24	3	312	CHL	CMD-C2D-C1D	6.70	136.53	124.71
24	3	304	CHL	CMD-C2D-C1D	6.70	136.53	124.71
25	u	307	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	p	310	CHL	C2C-C3C-C4C	-6.70	101.71	106.49
25	S	611	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	G	317	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	u	309	CHL	CMD-C2D-C1D	6.70	136.52	124.71
25	C	605	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	Y	317	CHL	C2C-C3C-C4C	-6.70	101.72	106.49
24	s	409	CHL	CMD-C2D-C1D	6.70	136.51	124.71
24	s	406	CHL	CMD-C2D-C1D	6.70	136.51	124.71
24	7	309	CHL	CMD-C2D-C1D	6.69	136.51	124.71
24	2	310	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
24	g	306	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
24	r	306	CHL	CMD-C2D-C1D	6.69	136.51	124.71
24	S	608	CHL	CMD-C2D-C1D	6.69	136.51	124.71
24	p	312	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
24	G	310	CHL	CMD-C2D-C1D	6.69	136.50	124.71
24	4	308	CHL	CMD-C2D-C1D	6.69	136.50	124.71
24	G	306	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
24	6	309	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
25	Y	307	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	n	315	CLA	C4A-NA-C1A	6.69	109.71	106.71
24	8	308	CHL	C2C-C3C-C4C	-6.68	101.72	106.49
24	S	605	CHL	CMD-C2D-C1D	6.68	136.49	124.71
25	9	315	CLA	C4A-NA-C1A	6.68	109.71	106.71
25	b	608	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	5	310	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
24	1	304	CHL	CMD-C2D-C1D	6.68	136.49	124.71
24	7	311	CHL	CMD-C2D-C1D	6.68	136.48	124.71
25	q	305	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	1	308	CHL	CMD-C2D-C1D	6.68	136.48	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	308	CHL	CMD-C2D-C1D	6.68	136.48	124.71
24	6	312	CHL	CMD-C2D-C1D	6.67	136.48	124.71
24	G	306	CHL	CMD-C2D-C1D	6.67	136.48	124.71
25	5	317	CLA	C4A-NA-C1A	6.67	109.71	106.71
25	g	317	CLA	C4A-NA-C1A	6.67	109.70	106.71
24	R	602	CHL	CMD-C2D-C1D	6.67	136.46	124.71
24	u	310	CHL	CMD-C2D-C1D	6.67	136.46	124.71
25	A	607	CLA	C4A-NA-C1A	6.67	109.70	106.71
24	7	313	CHL	CMD-C2D-C1D	6.66	136.46	124.71
24	N	304	CHL	CMD-C2D-C1D	6.66	136.45	124.71
25	C	608	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	S	606	CHL	CMD-C2D-C1D	6.66	136.45	124.71
24	y	318	CHL	C2C-C3C-C4C	-6.66	101.74	106.49
24	p	313	CHL	CMD-C2D-C1D	6.66	136.45	124.71
24	9	309	CHL	CMD-C2D-C1D	6.65	136.44	124.71
24	q	307	CHL	CMD-C2D-C1D	6.65	136.44	124.71
24	4	305	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
25	N	306	CLA	C4A-NA-C1A	6.65	109.70	106.71
24	6	308	CHL	CMD-C2D-C1D	6.65	136.43	124.71
24	s	414	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
24	n	304	CHL	CMD-C2D-C1D	6.65	136.43	124.71
31	a	608	8CT	C14-C13-C12	-6.65	117.82	127.31
25	S	616	CLA	C4A-NA-C1A	6.65	109.69	106.71
25	y	308	CLA	C4A-NA-C1A	6.65	109.69	106.71
24	2	309	CHL	CMD-C2D-C1D	6.65	136.43	124.71
24	2	318	CHL	CMD-C2D-C1D	6.64	136.42	124.71
24	5	309	CHL	CMD-C2D-C1D	6.64	136.42	124.71
24	6	309	CHL	CMD-C2D-C1D	6.64	136.42	124.71
25	4	306	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	p	311	CHL	CMD-C2D-C1D	6.64	136.42	124.71
24	9	310	CHL	CMD-C2D-C1D	6.64	136.42	124.71
24	r	303	CHL	CMD-C2D-C1D	6.64	136.42	124.71
24	7	310	CHL	CMD-C2D-C1D	6.64	136.42	124.71
25	Y	306	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	8	310	CHL	C2C-C3C-C4C	-6.64	101.76	106.49
24	R	601	CHL	CMD-C2D-C1D	6.64	136.41	124.71
24	g	312	CHL	CMD-C2D-C1D	6.64	136.41	124.71
25	Y	316	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	c	605	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	9	309	CHL	C2C-C3C-C4C	-6.64	101.76	106.49
25	5	307	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	u	311	CHL	CMD-C2D-C1D	6.63	136.41	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	307	CHL	CMD-C2D-C1D	6.63	136.40	124.71
25	R	604	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	b	602	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	3	310	CHL	CMD-C2D-C1D	6.63	136.39	124.71
25	n	314	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	5	318	CHL	CMD-C2D-C1D	6.62	136.39	124.71
31	s	415	8CT	C18-C17-C16	-6.62	117.86	127.31
25	9	306	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	8	303	CHL	CMD-C2D-C1D	6.62	136.38	124.71
24	q	309	CHL	C2C-C3C-C4C	-6.62	101.77	106.49
24	q	311	CHL	C2C-C3C-C4C	-6.62	101.77	106.49
24	q	303	CHL	CMD-C2D-C1D	6.62	136.38	124.71
25	B	605	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	4	314	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	r	302	CHL	CMD-C2D-C1D	6.62	136.38	124.71
24	S	608	CHL	C2C-C3C-C4C	-6.62	101.77	106.49
25	9	307	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	N	315	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	N	310	CHL	CMD-C2D-C1D	6.61	136.37	124.71
24	3	309	CHL	CMD-C2D-C1D	6.61	136.36	124.71
24	G	312	CHL	CMD-C2D-C1D	6.61	136.35	124.71
31	S	614	8CT	C18-C17-C16	-6.60	117.88	127.31
25	B	602	CLA	C4A-NA-C1A	6.60	109.67	106.71
25	9	316	CLA	C4A-NA-C1A	6.60	109.67	106.71
24	8	310	CHL	CMD-C2D-C1D	6.60	136.34	124.71
24	p	310	CHL	CMD-C2D-C1D	6.60	136.34	124.71
24	4	305	CHL	CMD-C2D-C1D	6.60	136.34	124.71
25	A	610	CLA	C4A-NA-C1A	6.60	109.67	106.71
25	6	307	CLA	C4A-NA-C1A	6.60	109.67	106.71
24	6	310	CHL	CMD-C2D-C1D	6.60	136.34	124.71
24	s	409	CHL	C2C-C3C-C4C	-6.60	101.79	106.49
25	1	313	CLA	C4A-NA-C1A	6.60	109.67	106.71
25	1	314	CLA	C4A-NA-C1A	6.60	109.67	106.71
25	r	314	CLA	C4A-NA-C1A	6.60	109.67	106.71
24	y	311	CHL	CMD-C2D-C1D	6.60	136.34	124.71
24	7	310	CHL	C2C-C3C-C4C	-6.60	101.79	106.49
25	q	312	CLA	C4A-NA-C1A	6.60	109.67	106.71
24	G	305	CHL	CMD-C2D-C1D	6.59	136.33	124.71
24	n	308	CHL	CMD-C2D-C1D	6.59	136.33	124.71
24	r	309	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
25	u	316	CLA	C4A-NA-C1A	6.59	109.67	106.71
25	r	312	CLA	C4A-NA-C1A	6.59	109.67	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	310	CHL	CMD-C2D-C1D	6.59	136.33	124.71
24	Y	319	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
24	s	414	CHL	CMD-C2D-C1D	6.59	136.33	124.71
25	2	308	CLA	C4A-NA-C1A	6.59	109.67	106.71
24	q	304	CHL	CMD-C2D-C1D	6.59	136.32	124.71
24	5	312	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
24	6	305	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
24	S	613	CHL	C2C-C3C-C4C	-6.58	101.80	106.49
24	g	305	CHL	CMD-C2D-C1D	6.58	136.31	124.71
25	s	413	CLA	C4A-NA-C1A	6.58	109.66	106.71
24	n	310	CHL	CMD-C2D-C1D	6.58	136.30	124.71
24	q	311	CHL	CMD-C2D-C1D	6.58	136.30	124.71
25	S	610	CLA	C4A-NA-C1A	6.58	109.66	106.71
24	G	318	CHL	CMD-C2D-C1D	6.57	136.30	124.71
24	s	407	CHL	CMD-C2D-C1D	6.57	136.30	124.71
25	8	305	CLA	C4A-NA-C1A	6.57	109.66	106.71
25	c	609	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	2	311	CHL	CMD-C2D-C1D	6.57	136.29	124.71
24	S	613	CHL	CMD-C2D-C1D	6.57	136.29	124.71
24	3	305	CHL	C2C-C3C-C4C	-6.57	101.81	106.49
25	3	307	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	8	304	CHL	CMD-C2D-C1D	6.56	136.28	124.71
24	6	305	CHL	CMD-C2D-C1D	6.56	136.28	124.71
25	n	313	CLA	C4A-NA-C1A	6.56	109.66	106.71
24	Y	311	CHL	CMD-C2D-C1D	6.56	136.28	124.71
24	g	311	CHL	CMD-C2D-C1D	6.56	136.28	124.71
27	r	316	XAT	O24-C25-C24	6.56	118.31	113.38
25	n	307	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	y	317	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	8	311	CLA	C4A-NA-C1A	6.56	109.65	106.71
25	s	417	CLA	C4A-NA-C1A	6.56	109.65	106.71
24	8	309	CHL	C2C-C3C-C4C	-6.56	101.81	106.49
24	g	318	CHL	CMD-C2D-C1D	6.56	136.27	124.71
31	C	613	8CT	C14-C13-C12	-6.55	117.96	127.31
25	R	613	CLA	C4A-NA-C1A	6.55	109.65	106.71
25	C	616	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	4	304	CHL	CMD-C2D-C1D	6.55	136.26	124.71
24	y	312	CHL	CMD-C2D-C1D	6.55	136.26	124.71
25	3	316	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	G	318	CHL	C2C-C3C-C4C	-6.55	101.82	106.49
25	c	616	CLA	C4A-NA-C1A	6.55	109.65	106.71
31	c	613	8CT	C14-C13-C12	-6.55	117.97	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	609	CLA	C4A-NA-C1A	6.54	109.65	106.71
24	5	310	CHL	CMD-C2D-C1D	6.54	136.24	124.71
24	Y	304	CHL	C2C-C3C-C4C	-6.54	101.83	106.49
24	2	310	CHL	CMD-C2D-C1D	6.53	136.23	124.71
24	R	605	CHL	C2C-C3C-C4C	-6.53	101.83	106.49
24	3	305	CHL	CMD-C2D-C1D	6.53	136.22	124.71
25	N	313	CLA	C4A-NA-C1A	6.53	109.64	106.71
25	y	307	CLA	C4A-NA-C1A	6.53	109.64	106.71
24	2	312	CHL	C2C-C3C-C4C	-6.53	101.84	106.49
25	B	608	CLA	C4A-NA-C1A	6.52	109.64	106.71
25	B	610	CLA	C4A-NA-C1A	6.52	109.64	106.71
25	c	608	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	q	310	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
25	g	314	CLA	C4A-NA-C1A	6.52	109.64	106.71
25	p	314	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	5	305	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
24	y	305	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
27	R	615	XAT	C18-C5-C6	-6.52	111.34	122.26
24	u	310	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
25	8	312	CLA	C4A-NA-C1A	6.51	109.64	106.71
25	N	307	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	9	313	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	y	318	CHL	CMD-C2D-C1D	6.51	136.19	124.71
25	6	316	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	1	306	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	s	410	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	n	316	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	1	310	CHL	CMD-C2D-C1D	6.50	136.17	124.71
25	N	314	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	r	305	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	q	309	CHL	CMD-C2D-C1D	6.50	136.17	124.71
25	a	610	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	2	317	CLA	C4A-NA-C1A	6.49	109.63	106.71
25	s	405	CLA	C4A-NA-C1A	6.49	109.63	106.71
25	D	404	CLA	C4A-NA-C1A	6.49	109.62	106.71
25	S	604	CLA	C4A-NA-C1A	6.49	109.62	106.71
25	5	308	CLA	C4A-NA-C1A	6.49	109.62	106.71
27	r	316	XAT	C18-C5-C6	-6.49	111.38	122.26
24	4	310	CHL	CMD-C2D-C1D	6.49	136.14	124.71
25	Y	313	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	5	311	CHL	CMD-C2D-C1D	6.48	136.14	124.71
24	Y	317	CHL	CMD-C2D-C1D	6.48	136.13	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	318	CHL	CMD-C2D-C1D	6.48	136.13	124.71
25	B	615	CLA	C4A-NA-C1A	6.47	109.62	106.71
25	1	316	CLA	C4A-NA-C1A	6.47	109.62	106.71
31	T	101	8CT	C14-C13-C12	-6.47	118.07	127.31
24	R	608	CHL	C2C-C3C-C4C	-6.47	101.88	106.49
24	s	407	CHL	C2C-C3C-C4C	-6.47	101.88	106.49
24	7	318	CHL	CMD-C2D-C1D	6.47	136.12	124.71
24	q	307	CHL	C2C-C3C-C4C	-6.47	101.88	106.49
31	t	101	8CT	C14-C13-C12	-6.47	118.08	127.31
25	2	307	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	S	612	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	G	307	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	N	316	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	C	603	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	q	315	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	b	610	CLA	C4A-NA-C1A	6.47	109.61	106.71
24	g	318	CHL	C2C-C3C-C4C	-6.46	101.88	106.49
25	R	612	CLA	C4A-NA-C1A	6.46	109.61	106.71
25	G	314	CLA	C4A-NA-C1A	6.46	109.61	106.71
24	R	606	CHL	CMD-C2D-C1D	6.46	136.09	124.71
24	N	312	CHL	C2C-C3C-C4C	-6.46	101.89	106.49
24	1	305	CHL	CMD-C2D-C1D	6.46	136.09	124.71
25	g	308	CLA	C4A-NA-C1A	6.45	109.61	106.71
25	4	313	CLA	C4A-NA-C1A	6.45	109.61	106.71
25	b	603	CLA	C4A-NA-C1A	6.45	109.61	106.71
24	p	318	CHL	C2C-C3C-C4C	-6.45	101.89	106.49
24	n	312	CHL	C2C-C3C-C4C	-6.45	101.89	106.49
24	7	313	CHL	C2C-C3C-C4C	-6.45	101.89	106.49
25	c	603	CLA	C4A-NA-C1A	6.45	109.60	106.71
25	u	308	CLA	C4A-NA-C1A	6.44	109.60	106.71
24	9	305	CHL	CMD-C2D-C1D	6.44	136.06	124.71
25	b	614	CLA	C4A-NA-C1A	6.44	109.60	106.71
25	B	612	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	1	310	CHL	C2C-C3C-C4C	-6.43	101.91	106.49
25	R	611	CLA	C4A-NA-C1A	6.43	109.60	106.71
25	y	314	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	R	601	CHL	C2C-C3C-C4C	-6.43	101.91	106.49
24	4	312	CHL	CMD-C2D-C1D	6.43	136.04	124.71
25	5	314	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	b	615	CLA	C4A-NA-C1A	6.42	109.59	106.71
24	2	305	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
25	g	307	CLA	C4A-NA-C1A	6.41	109.59	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	315	CLA	C4A-NA-C1A	6.41	109.59	106.71
24	S	606	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
25	s	404	CLA	C4A-NA-C1A	6.41	109.59	106.71
24	u	306	CHL	CMD-C2D-C1D	6.41	136.00	124.71
24	2	306	CHL	CMD-C2D-C1D	6.41	136.00	124.71
25	7	314	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	r	306	CHL	C2C-C3C-C4C	-6.40	101.92	106.49
25	B	603	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	n	311	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
25	8	306	CLA	C4A-NA-C1A	6.40	109.58	106.71
25	7	308	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	G	310	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
24	g	312	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
31	S	614	8CT	C14-C13-C12	-6.40	118.18	127.31
24	S	605	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
24	R	608	CHL	CMD-C2D-C1D	6.39	135.98	124.71
25	B	614	CLA	C4A-NA-C1A	6.39	109.58	106.71
24	r	307	CHL	CMD-C2D-C1D	6.39	135.97	124.71
24	s	406	CHL	C2C-C3C-C4C	-6.39	101.94	106.49
24	1	312	CHL	CMD-C2D-C1D	6.39	135.97	124.71
25	C	606	CLA	C4A-NA-C1A	6.38	109.57	106.71
25	4	316	CLA	C4A-NA-C1A	6.38	109.57	106.71
25	6	314	CLA	C4A-NA-C1A	6.38	109.57	106.71
24	Y	312	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
24	p	313	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
24	N	308	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
24	g	311	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
24	8	307	CHL	C2C-C3C-C4C	-6.37	101.94	106.49
24	g	310	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
24	6	310	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
24	7	318	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
25	G	315	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	u	314	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	4	310	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
24	7	306	CHL	CMD-C2D-C1D	6.37	135.94	124.71
24	N	311	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
25	q	313	CLA	C4A-NA-C1A	6.37	109.57	106.71
31	s	415	8CT	C14-C13-C12	-6.36	118.23	127.31
25	S	609	CLA	C4A-NA-C1A	6.36	109.56	106.71
27	R	615	XAT	O24-C25-C24	6.36	118.16	113.38
24	3	304	CHL	C2C-C3C-C4C	-6.35	101.96	106.49
25	3	306	CLA	C4A-NA-C1A	6.35	109.56	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	606	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	y	313	CHL	C2C-C3C-C4C	-6.35	101.96	106.49
24	6	304	CHL	C2C-C3C-C4C	-6.35	101.96	106.49
24	G	311	CHL	C2C-C3C-C4C	-6.35	101.96	106.49
24	y	309	CHL	C2C-C3C-C4C	-6.35	101.96	106.49
25	R	610	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	5	306	CHL	CMD-C2D-C1D	6.35	135.90	124.71
25	q	306	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	Y	308	CHL	C2C-C3C-C4C	-6.35	101.97	106.49
29	4	301	0UR	C14-C15-C16	-6.34	118.26	127.31
25	p	308	CLA	C4A-NA-C1A	6.34	109.56	106.71
28	p	304	NEX	C11-C12-C13	-6.34	108.61	126.42
24	u	305	CHL	C2C-C3C-C4C	-6.34	101.97	106.49
29	1	301	0UR	C14-C15-C16	-6.34	118.27	127.31
25	6	313	CLA	C4A-NA-C1A	6.34	109.56	106.71
28	r	317	NEX	C11-C12-C13	-6.33	108.63	126.42
28	g	304	NEX	C11-C12-C13	-6.33	108.63	126.42
28	5	304	NEX	C11-C12-C13	-6.33	108.64	126.42
28	7	304	NEX	C11-C12-C13	-6.33	108.64	126.42
24	1	311	CHL	C2C-C3C-C4C	-6.33	101.98	106.49
25	2	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
28	u	304	NEX	C11-C12-C13	-6.33	108.64	126.42
25	y	315	CLA	C4A-NA-C1A	6.33	109.55	106.71
28	2	304	NEX	C11-C12-C13	-6.33	108.65	126.42
24	N	310	CHL	C2C-C3C-C4C	-6.32	101.98	106.49
24	u	311	CHL	C2C-C3C-C4C	-6.32	101.98	106.49
28	R	616	NEX	C11-C12-C13	-6.32	108.66	126.42
28	S	617	NEX	C11-C12-C13	-6.32	108.66	126.42
24	r	309	CHL	CMD-C2D-C1D	6.32	135.85	124.71
28	4	303	NEX	C11-C12-C13	-6.32	108.66	126.42
28	y	304	NEX	C11-C12-C13	-6.32	108.67	126.42
24	9	304	CHL	C2C-C3C-C4C	-6.32	101.99	106.49
24	9	310	CHL	C2C-C3C-C4C	-6.32	101.99	106.49
28	G	304	NEX	C11-C12-C13	-6.32	108.67	126.42
28	1	303	NEX	C11-C12-C13	-6.31	108.68	126.42
28	9	319	NEX	C11-C12-C13	-6.31	108.68	126.42
25	S	603	CLA	C4A-NA-C1A	6.31	109.55	106.71
24	4	309	CHL	C2C-C3C-C4C	-6.31	101.99	106.49
25	b	613	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	Y	314	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	6	306	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	4	307	CLA	C4A-NA-C1A	6.31	109.54	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	309	CHL	C2C-C3C-C4C	-6.31	101.99	106.49
25	G	308	CLA	C4A-NA-C1A	6.30	109.54	106.71
24	n	308	CHL	C2C-C3C-C4C	-6.30	102.00	106.49
24	7	311	CHL	C2C-C3C-C4C	-6.30	102.00	106.49
25	C	610	CLA	C4A-NA-C1A	6.30	109.54	106.71
24	3	317	CHL	C2C-C3C-C4C	-6.30	102.00	106.49
24	2	318	CHL	C2C-C3C-C4C	-6.29	102.00	106.49
24	G	312	CHL	C2C-C3C-C4C	-6.29	102.00	106.49
24	n	310	CHL	C2C-C3C-C4C	-6.29	102.01	106.49
24	p	306	CHL	CMD-C2D-C1D	6.28	135.79	124.71
24	G	313	CHL	C2C-C3C-C4C	-6.28	102.01	106.49
24	7	309	CHL	CHB-C1B-NB	-6.28	117.61	124.26
25	8	314	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	5	313	CHL	C2C-C3C-C4C	-6.28	102.01	106.49
25	A	604	CLA	C4A-NA-C1A	6.27	109.53	106.71
24	5	311	CHL	C2C-C3C-C4C	-6.27	102.02	106.49
25	r	311	CLA	C4A-NA-C1A	6.27	109.52	106.71
24	1	312	CHL	C2C-C3C-C4C	-6.26	102.03	106.49
24	6	317	CHL	C2C-C3C-C4C	-6.25	102.03	106.49
24	g	305	CHL	C2C-C3C-C4C	-6.25	102.03	106.49
24	r	302	CHL	C2C-C3C-C4C	-6.25	102.03	106.49
25	3	313	CLA	C4A-NA-C1A	6.25	109.52	106.71
24	4	311	CHL	C2C-C3C-C4C	-6.25	102.03	106.49
24	3	310	CHL	C2C-C3C-C4C	-6.24	102.04	106.49
24	Y	305	CHL	CMD-C2D-C1D	6.24	135.71	124.71
24	2	309	CHL	C2C-C3C-C4C	-6.23	102.05	106.49
24	G	305	CHL	C2C-C3C-C4C	-6.23	102.05	106.49
24	5	309	CHL	C2C-C3C-C4C	-6.23	102.05	106.49
25	c	610	CLA	C4A-NA-C1A	6.22	109.50	106.71
24	4	312	CHL	C2C-C3C-C4C	-6.22	102.06	106.49
24	5	318	CHL	C2C-C3C-C4C	-6.22	102.06	106.49
24	y	306	CHL	CMD-C2D-C1D	6.22	135.67	124.71
24	2	313	CHL	C2C-C3C-C4C	-6.22	102.06	106.49
24	n	305	CHL	CMD-C2D-C1D	6.22	135.67	124.71
24	q	316	CHL	C2C-C3C-C4C	-6.22	102.06	106.49
35	d	403	PHO	C4D-CHA-CBD	-6.21	105.71	108.52
24	4	308	CHL	C2C-C3C-C4C	-6.21	102.06	106.49
24	1	308	CHL	C2C-C3C-C4C	-6.20	102.07	106.49
25	B	613	CLA	C4A-NA-C1A	6.20	109.49	106.71
24	9	311	CHL	C2C-C3C-C4C	-6.20	102.07	106.49
24	p	309	CHL	CHB-C1B-NB	-6.20	117.69	124.26
35	a	606	PHO	C4D-CHA-CBD	-6.19	105.72	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	312	CHL	C2C-C3C-C4C	-6.19	102.08	106.49
24	8	315	CHL	C2C-C3C-C4C	-6.19	102.08	106.49
25	b	612	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	N	305	CHL	CMD-C2D-C1D	6.18	135.61	124.71
25	1	307	CLA	C4A-NA-C1A	6.18	109.48	106.71
25	3	314	CLA	C4A-NA-C1A	6.18	109.48	106.71
24	N	317	CHL	C2C-C3C-C4C	-6.18	102.08	106.49
24	u	318	CHL	C2C-C3C-C4C	-6.18	102.09	106.49
24	1	304	CHL	C2C-C3C-C4C	-6.18	102.09	106.49
24	p	305	CHL	C2C-C3C-C4C	-6.18	102.09	106.49
35	D	403	PHO	C4D-CHA-CBD	-6.17	105.72	108.52
24	G	309	CHL	CHB-C1B-NB	-6.17	117.72	124.26
24	4	304	CHL	C2C-C3C-C4C	-6.17	102.09	106.49
24	n	317	CHL	C2C-C3C-C4C	-6.17	102.09	106.49
24	9	308	CHL	C2C-C3C-C4C	-6.17	102.09	106.49
24	9	317	CHL	C2C-C3C-C4C	-6.16	102.09	106.49
24	g	313	CHL	C2C-C3C-C4C	-6.16	102.09	106.49
24	7	309	CHL	C1D-ND-C4D	6.16	110.71	106.33
24	N	317	CHL	C1D-ND-C4D	6.16	110.71	106.33
24	2	311	CHL	C2C-C3C-C4C	-6.16	102.10	106.49
24	n	317	CHL	C1D-ND-C4D	6.16	110.71	106.33
24	u	313	CHL	C2C-C3C-C4C	-6.16	102.10	106.49
24	9	317	CHL	CHB-C1B-NB	-6.16	117.74	124.26
24	u	318	CHL	CHB-C1B-NB	-6.15	117.74	124.26
25	A	605	CLA	C4A-NA-C1A	6.15	109.47	106.71
24	u	309	CHL	C2C-C3C-C4C	-6.15	102.11	106.49
24	3	312	CHL	C2C-C3C-C4C	-6.14	102.11	106.49
24	p	311	CHL	C2C-C3C-C4C	-6.14	102.11	106.49
24	N	304	CHL	C2C-C3C-C4C	-6.13	102.12	106.49
24	N	317	CHL	CHB-C1B-NB	-6.13	117.77	124.26
24	3	308	CHL	C2C-C3C-C4C	-6.13	102.12	106.49
24	6	312	CHL	C2C-C3C-C4C	-6.13	102.12	106.49
24	6	308	CHL	C2C-C3C-C4C	-6.12	102.12	106.49
24	7	305	CHL	C2C-C3C-C4C	-6.12	102.13	106.49
28	7	304	NEX	C38-C25-C26	-6.11	112.02	122.26
28	4	303	NEX	C38-C25-C26	-6.11	112.02	122.26
25	a	605	CLA	C4A-NA-C1A	6.11	109.45	106.71
31	X	601	8CT	C18-C17-C16	-6.11	118.59	127.31
31	b	617	8CT	C19-C20-C21	-6.11	118.59	127.31
25	a	604	CLA	C4A-NA-C1A	6.11	109.45	106.71
24	u	312	CHL	C2C-C3C-C4C	-6.11	102.14	106.49
28	G	304	NEX	C38-C25-C26	-6.10	112.04	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	617	NEX	C38-C25-C26	-6.10	112.04	122.26
28	u	304	NEX	C38-C25-C26	-6.09	112.05	122.26
28	5	304	NEX	C38-C25-C26	-6.09	112.05	122.26
28	p	304	NEX	C38-C25-C26	-6.09	112.05	122.26
24	1	317	CHL	CHB-C1B-NB	-6.09	117.81	124.26
28	2	304	NEX	C38-C25-C26	-6.08	112.07	122.26
35	A	606	PHO	C4D-CHA-CBD	-6.08	105.77	108.52
24	n	304	CHL	C2C-C3C-C4C	-6.07	102.16	106.49
28	9	319	NEX	C38-C25-C26	-6.07	112.08	122.26
28	y	304	NEX	C38-C25-C26	-6.07	112.08	122.26
24	g	309	CHL	C2C-C3C-C4C	-6.07	102.16	106.49
28	g	304	NEX	C38-C25-C26	-6.07	112.08	122.26
24	g	309	CHL	CHB-C1B-NB	-6.07	117.84	124.26
24	n	317	CHL	CHB-C1B-NB	-6.06	117.84	124.26
28	1	303	NEX	C38-C25-C26	-6.06	112.10	122.26
24	4	317	CHL	CHB-C1B-NB	-6.06	117.84	124.26
31	B	617	8CT	C19-C20-C21	-6.06	118.67	127.31
28	R	616	NEX	C38-C25-C26	-6.06	112.11	122.26
31	S	614	8CT	C04-C03-C02	-6.05	114.09	122.61
24	9	308	CHL	CHB-C1B-NB	-6.05	117.85	124.26
28	r	317	NEX	C38-C25-C26	-6.04	112.13	122.26
24	p	309	CHL	C1D-ND-C4D	6.03	110.62	106.33
31	V	401	8CT	C10-C11-C12	-6.03	117.13	126.23
24	1	304	CHL	CHB-C1B-NB	-6.02	117.88	124.26
24	q	303	CHL	C2C-C3C-C4C	-6.02	102.20	106.49
29	4	301	0UR	C10-C11-C12	-6.02	118.72	127.31
24	u	318	CHL	C1D-ND-C4D	6.01	110.61	106.33
24	4	304	CHL	CHB-C1B-NB	-6.01	117.89	124.26
24	G	309	CHL	C2C-C3C-C4C	-6.01	102.20	106.49
31	s	415	8CT	C04-C03-C02	-6.00	114.16	122.61
24	4	317	CHL	C2C-C3C-C4C	-6.00	102.22	106.49
31	x	601	8CT	C18-C17-C16	-5.99	118.77	127.31
24	1	317	CHL	C2C-C3C-C4C	-5.98	102.22	106.49
31	v	401	8CT	C10-C11-C12	-5.98	117.20	126.23
24	p	309	CHL	C2C-C3C-C4C	-5.98	102.22	106.49
24	1	308	CHL	CHB-C1B-NB	-5.98	117.93	124.26
24	7	309	CHL	C2C-C3C-C4C	-5.97	102.23	106.49
24	1	304	CHL	C1D-ND-C4D	5.97	110.58	106.33
24	8	303	CHL	C2C-C3C-C4C	-5.96	102.24	106.49
24	G	309	CHL	C1D-ND-C4D	5.95	110.56	106.33
24	4	304	CHL	C1D-ND-C4D	5.95	110.56	106.33
31	S	614	8CT	C30-C31-C32	-5.95	114.15	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	308	CHL	CHB-C1B-NB	-5.95	117.96	124.26
24	9	317	CHL	C1D-ND-C4D	5.93	110.55	106.33
24	g	309	CHL	C1D-ND-C4D	5.93	110.55	106.33
31	s	415	8CT	C30-C31-C32	-5.92	114.18	121.47
24	u	309	CHL	CHB-C1B-NB	-5.92	118.00	124.26
24	8	315	CHL	CHB-C1B-NB	-5.90	118.01	124.26
24	q	316	CHL	CHB-C1B-NB	-5.90	118.01	124.26
29	1	301	0UR	C10-C11-C12	-5.87	118.93	127.31
24	2	318	CHL	CHB-C1B-NB	-5.86	118.06	124.26
24	5	318	CHL	CHB-C1B-NB	-5.85	118.06	124.26
24	6	308	CHL	CHB-C1B-NB	-5.84	118.08	124.26
24	9	308	CHL	C1D-ND-C4D	5.83	110.48	106.33
31	B	617	8CT	C18-C17-C16	-5.81	119.01	127.31
24	4	317	CHL	C1D-ND-C4D	5.79	110.45	106.33
24	3	308	CHL	CHB-C1B-NB	-5.78	118.13	124.26
31	s	416	8CT	C01-C02-C03	-5.78	118.03	124.53
24	s	403	CHL	CMD-C2D-C1D	5.78	134.90	124.71
24	n	308	CHL	CHB-C1B-NB	-5.78	118.14	124.26
31	C	614	8CT	C14-C13-C12	-5.78	119.07	127.31
24	S	602	CHL	CMD-C2D-C1D	5.77	134.89	124.71
31	T	101	8CT	C01-C02-C03	-5.75	118.07	124.53
31	c	614	8CT	C14-C13-C12	-5.74	119.11	127.31
24	p	306	CHL	CHD-C4C-C3C	-5.74	116.40	124.84
24	7	306	CHL	CHD-C4C-C3C	-5.74	116.41	124.84
24	Y	309	CHL	CHD-C4C-C3C	-5.73	116.41	124.84
24	7	312	CHL	CHD-C4C-C3C	-5.73	116.41	124.84
31	B	617	8CT	C35-C30-C29	-5.73	105.45	112.70
31	b	617	8CT	C35-C30-C29	-5.73	105.46	112.70
31	T	101	8CT	C18-C17-C16	-5.72	119.14	127.31
24	5	309	CHL	CHB-C1B-NB	-5.72	118.20	124.26
31	t	101	8CT	C18-C17-C16	-5.72	119.15	127.31
24	1	317	CHL	C1D-ND-C4D	5.71	110.39	106.33
31	b	617	8CT	C18-C17-C16	-5.70	119.17	127.31
24	5	318	CHL	C1D-ND-C4D	5.70	110.39	106.33
24	3	308	CHL	C1D-ND-C4D	5.69	110.38	106.33
31	t	101	8CT	C01-C02-C03	-5.69	118.14	124.53
24	u	313	CHL	C1D-ND-C4D	5.69	110.37	106.33
24	6	308	CHL	C1D-ND-C4D	5.68	110.37	106.33
24	u	309	CHL	C1D-ND-C4D	5.68	110.37	106.33
24	u	305	CHL	CHB-C1B-NB	-5.67	118.26	124.26
24	p	312	CHL	CHD-C4C-C3C	-5.67	116.51	124.84
24	9	312	CHL	C1D-ND-C4D	5.66	110.36	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	308	CHL	C1D-ND-C4D	5.66	110.36	106.33
24	1	308	CHL	C1D-ND-C4D	5.65	110.35	106.33
31	S	615	8CT	C01-C02-C03	-5.65	118.19	124.53
24	y	310	CHL	CHD-C4C-C3C	-5.64	116.55	124.84
31	t	101	8CT	C24-C25-C26	-5.62	119.29	127.31
24	2	318	CHL	C1D-ND-C4D	5.62	110.33	106.33
24	8	315	CHL	C1D-ND-C4D	5.62	110.33	106.33
24	2	309	CHL	CHB-C1B-NB	-5.61	118.31	124.26
24	q	316	CHL	C1D-ND-C4D	5.61	110.32	106.33
31	s	416	8CT	C39-C16-C17	-5.60	115.08	122.92
31	S	615	8CT	C39-C16-C17	-5.59	115.10	122.92
24	8	303	CHL	CHB-C1B-NB	-5.58	118.35	124.26
31	d	410	8CT	C14-C13-C12	-5.57	119.35	127.31
24	Y	310	CHL	C3B-C2B-C1B	-5.57	100.44	107.16
24	R	601	CHL	CHB-C1B-NB	-5.57	118.36	124.26
24	S	607	CHL	C3B-C2B-C1B	-5.57	100.44	107.16
24	Y	304	CHL	CHD-C4C-C3C	-5.56	116.67	124.84
24	y	305	CHL	CHD-C4C-C3C	-5.56	116.67	124.84
24	y	311	CHL	C3B-C2B-C1B	-5.55	100.46	107.16
24	s	414	CHL	O2D-CGD-CBD	5.54	121.11	111.27
24	7	306	CHL	C2A-C1A-CHA	-5.54	114.17	123.86
36	A	611	BCT	O2-C-O1	5.54	133.91	119.55
24	y	318	CHL	C3B-C2B-C1B	-5.53	100.48	107.16
24	n	309	CHL	C2A-C1A-CHA	-5.53	114.19	123.86
24	s	408	CHL	C3B-C2B-C1B	-5.52	100.49	107.16
24	Y	309	CHL	C2A-C1A-CHA	-5.52	114.20	123.86
24	5	309	CHL	C1D-ND-C4D	5.52	110.26	106.33
24	S	601	CHL	C3B-C2B-C1B	-5.52	100.50	107.16
24	R	605	CHL	CHD-C4C-C3C	-5.52	116.73	124.84
24	s	402	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
36	a	611	BCT	O2-C-O1	5.50	133.82	119.55
24	G	313	CHL	C1D-ND-C4D	5.49	110.24	106.33
24	q	303	CHL	CHB-C1B-NB	-5.49	118.44	124.26
24	3	317	CHL	O2D-CGD-CBD	5.49	121.02	111.27
24	S	613	CHL	O2D-CGD-CBD	5.49	121.02	111.27
24	Y	317	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
24	S	602	CHL	CHD-C4C-C3C	-5.48	116.78	124.84
24	r	302	CHL	CHB-C1B-NB	-5.48	118.45	124.26
24	g	313	CHL	C1D-ND-C4D	5.48	110.22	106.33
24	p	306	CHL	C2A-C1A-CHA	-5.47	114.29	123.86
24	8	303	CHL	C1D-ND-C4D	5.46	110.22	106.33
24	5	309	CHL	C3B-C2B-C1B	-5.46	100.57	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	v	401	8CT	C19-C20-C21	-5.46	119.52	127.31
31	V	401	8CT	C19-C20-C21	-5.45	119.53	127.31
24	2	309	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
24	n	308	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
29	5	301	0UR	C14-C15-C16	-5.45	119.54	127.31
24	R	607	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
24	s	403	CHL	CHD-C4C-C3C	-5.44	116.84	124.84
29	2	301	0UR	C14-C15-C16	-5.44	119.54	127.31
24	3	317	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
31	a	608	8CT	C18-C17-C16	-5.44	119.55	127.31
31	T	101	8CT	C24-C25-C26	-5.44	119.55	127.31
24	6	310	CHL	C1D-ND-C4D	5.43	110.19	106.33
24	3	308	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
24	n	308	CHL	C1D-ND-C4D	5.43	110.19	106.33
24	9	310	CHL	CHB-C1B-NB	-5.43	118.51	124.26
24	q	307	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
24	p	309	CHL	C3B-C2B-C1B	-5.42	100.61	107.16
24	R	606	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	u	305	CHL	C1D-ND-C4D	5.42	110.19	106.33
24	R	605	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	2	312	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	4	308	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	6	308	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	Y	305	CHL	CHD-C4C-C3C	-5.41	116.88	124.84
24	2	309	CHL	C1D-ND-C4D	5.41	110.18	106.33
24	7	305	CHL	CHD-C4C-C3C	-5.41	116.89	124.84
24	6	317	CHL	O2D-CGD-CBD	5.41	120.88	111.27
24	R	601	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
24	1	308	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
24	r	308	CHL	C3B-C2B-C1B	-5.41	100.64	107.16
24	r	302	CHL	C3B-C2B-C1B	-5.41	100.64	107.16
24	g	311	CHL	CHB-C1B-NB	-5.40	118.53	124.26
24	5	312	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	7	318	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	6	312	CHL	C1D-ND-C4D	5.40	110.17	106.33
24	G	311	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	6	317	CHL	CHB-C1B-NB	-5.40	118.54	124.26
24	8	307	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	g	318	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	Y	311	CHL	CHD-C4C-C3C	-5.40	116.90	124.84
24	u	311	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	7	311	CHL	O2D-CGD-CBD	5.40	120.86	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	303	CHL	C1D-ND-C4D	5.40	110.17	106.33
24	r	302	CHL	O2D-CGD-CBD	5.40	120.86	111.27
24	6	317	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
24	p	318	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
24	2	305	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
24	9	317	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
24	n	304	CHL	C1D-ND-C4D	5.38	110.16	106.33
24	1	312	CHL	O2D-CGD-CBD	5.38	120.83	111.27
24	1	305	CHL	C3B-C2B-C1B	-5.38	100.66	107.16
24	7	305	CHL	C2A-C1A-CHA	-5.38	114.45	123.86
24	p	305	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
24	7	309	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
31	A	608	8CT	C18-C17-C16	-5.38	119.63	127.31
24	2	318	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	N	308	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	Y	305	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	g	311	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	y	306	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	Y	308	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	s	406	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	4	317	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
24	p	305	CHL	C2A-C1A-CHA	-5.37	114.48	123.86
24	n	304	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	S	605	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	9	310	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	8	315	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	N	304	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	7	305	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	p	310	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	3	317	CHL	CHB-C1B-NB	-5.36	118.58	124.26
24	n	309	CHL	CHD-C4C-C3C	-5.36	116.96	124.84
24	9	311	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	y	309	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	p	305	CHL	CHD-C4C-C3C	-5.36	116.97	124.84
24	u	312	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	7	312	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	5	305	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	p	312	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	u	318	CHL	C3B-C2B-C1B	-5.36	100.70	107.16
24	R	601	CHL	O2D-CGD-CBD	5.36	120.78	111.27
24	9	310	CHL	C1D-ND-C4D	5.35	110.14	106.33
24	y	310	CHL	C2A-C1A-CHA	-5.35	114.50	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	318	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
27	R	615	XAT	O24-C25-C38	5.35	121.47	115.06
24	9	312	CHL	CHB-C1B-NB	-5.35	118.59	124.26
24	4	312	CHL	O2D-CGD-CBD	5.35	120.78	111.27
24	n	317	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
24	n	310	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
24	y	312	CHL	CHD-C4C-C3C	-5.35	116.98	124.84
24	N	304	CHL	C1D-ND-C4D	5.35	110.13	106.33
24	6	304	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
24	n	305	CHL	O2D-CGD-CBD	5.35	120.77	111.27
24	g	310	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
24	7	310	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
24	u	311	CHL	CHB-C1B-NB	-5.34	118.60	124.26
24	n	304	CHL	CHB-C1B-NB	-5.34	118.60	124.26
24	5	318	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
24	y	306	CHL	CHD-C4C-C3C	-5.34	116.98	124.84
24	Y	304	CHL	C2A-C1A-CHA	-5.34	114.52	123.86
24	N	309	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
24	3	312	CHL	C1D-ND-C4D	5.34	110.13	106.33
24	R	601	CHL	C1D-ND-C4D	5.34	110.13	106.33
24	N	310	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
24	p	306	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
24	q	308	CHL	O2D-CGD-CBD	5.34	120.75	111.27
24	n	309	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
27	r	316	XAT	O24-C25-C38	5.34	121.45	115.06
24	N	317	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
24	r	307	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
31	C	613	8CT	C18-C17-C16	-5.33	119.70	127.31
24	y	305	CHL	C2A-C1A-CHA	-5.33	114.54	123.86
24	u	305	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
24	8	309	CHL	CHD-C4C-C3C	-5.33	117.01	124.84
24	3	310	CHL	C1D-ND-C4D	5.33	110.12	106.33
24	G	305	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
24	u	312	CHL	CHB-C1B-NB	-5.33	118.62	124.26
24	5	306	CHL	C3B-C2B-C1B	-5.32	100.73	107.16
24	Y	310	CHL	CHD-C4C-C3C	-5.32	117.02	124.84
24	N	312	CHL	O2D-CGD-CBD	5.32	120.73	111.27
24	s	414	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
24	N	304	CHL	CHB-C1B-NB	-5.32	118.62	124.26
24	R	607	CHL	CHD-C4C-C3C	-5.32	117.02	124.84
24	2	310	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
24	u	313	CHL	C3B-C2B-C1B	-5.32	100.74	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	602	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	S	613	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	Y	311	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	4	305	CHL	O2D-CGD-CBD	5.31	120.71	111.27
24	5	310	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	r	303	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	q	316	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	2	306	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	1	317	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	G	310	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	1	305	CHL	O2D-CGD-CBD	5.31	120.70	111.27
24	u	313	CHL	CHB-C1B-NB	-5.30	118.64	124.26
24	4	305	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
24	g	309	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
31	c	613	8CT	C18-C17-C16	-5.30	119.74	127.31
24	u	309	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
24	r	302	CHL	C1D-ND-C4D	5.30	110.10	106.33
24	7	306	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
24	Y	317	CHL	CHD-C4C-C3C	-5.29	117.06	124.84
24	G	309	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
31	v	401	8CT	C01-C02-C03	-5.29	118.58	124.53
24	3	312	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
24	n	312	CHL	O2D-CGD-CBD	5.29	120.67	111.27
24	4	304	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
31	C	615	8CT	C01-C02-C03	-5.29	118.59	124.53
24	S	606	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
24	9	304	CHL	C3B-C2B-C1B	-5.28	100.78	107.16
24	R	606	CHL	O2D-CGD-CBD	5.28	120.66	111.27
24	y	312	CHL	C3B-C2B-C1B	-5.28	100.78	107.16
24	q	308	CHL	C3B-C2B-C1B	-5.28	100.78	107.16
24	n	311	CHL	CHD-C4C-C3C	-5.28	117.08	124.84
24	9	308	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
24	r	308	CHL	CHD-C4C-C3C	-5.28	117.08	124.84
24	3	310	CHL	CHB-C1B-NB	-5.28	118.67	124.26
31	c	614	8CT	C18-C17-C16	-5.28	119.78	127.31
24	G	312	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
24	4	312	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
24	6	310	CHL	CHB-C1B-NB	-5.28	118.67	124.26
24	q	309	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
24	8	309	CHL	C2A-C1A-CHA	-5.27	114.64	123.86
24	Y	319	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
24	g	305	CHL	C3B-C2B-C1B	-5.27	100.80	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	318	CHL	CHD-C4C-C3C	-5.27	117.09	124.84
24	r	303	CHL	O2D-CGD-CBD	5.27	120.63	111.27
24	3	304	CHL	C3B-C2B-C1B	-5.27	100.81	107.16
24	1	312	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
24	p	311	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
24	3	310	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
24	7	311	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
24	6	312	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
24	r	306	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
24	5	306	CHL	CHD-C4C-C3C	-5.26	117.11	124.84
24	7	305	CHL	O2D-CGD-CBD	5.26	120.61	111.27
24	8	308	CHL	O2D-CGD-CBD	5.26	120.61	111.27
31	V	401	8CT	C01-C02-C03	-5.25	118.63	124.53
24	R	608	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
24	N	311	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
24	q	310	CHL	CHD-C4C-C3C	-5.25	117.12	124.84
24	9	311	CHL	CHB-C1B-NB	-5.25	118.70	124.26
24	1	304	CHL	C3B-C2B-C1B	-5.25	100.83	107.16
24	g	306	CHL	C2A-C1A-CHA	-5.25	114.68	123.86
24	r	309	CHL	C3B-C2B-C1B	-5.25	100.83	107.16
24	N	309	CHL	C2A-C1A-CHA	-5.25	114.69	123.86
24	7	306	CHL	O2D-CGD-CBD	5.25	120.59	111.27
24	9	312	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
24	s	407	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
24	N	312	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
24	N	309	CHL	CHD-C4C-C3C	-5.24	117.14	124.84
24	3	305	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
24	7	309	CHL	C4A-NA-C1A	5.24	109.06	106.71
24	R	602	CHL	O2D-CGD-CBD	5.24	120.57	111.27
24	R	605	CHL	C2A-C1A-CHA	-5.24	114.71	123.85
31	C	614	8CT	C18-C17-C16	-5.24	119.84	127.31
24	q	308	CHL	C2A-C1A-CHA	-5.23	114.71	123.86
24	N	305	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
24	u	311	CHL	C1D-ND-C4D	5.23	110.05	106.33
24	6	310	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
24	q	303	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
24	r	307	CHL	O2D-CGD-CBD	5.23	120.56	111.27
24	4	310	CHL	C3B-C2B-C1B	-5.22	100.85	107.16
24	Y	308	CHL	CHB-C1B-NB	-5.22	118.73	124.26
24	8	307	CHL	O2D-CGD-CBD	5.22	120.55	111.27
24	s	408	CHL	CHD-C4C-C3C	-5.22	117.17	124.84
24	6	305	CHL	C3B-C2B-C1B	-5.22	100.86	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	306	CHL	O2D-CGD-CBD	5.22	120.54	111.27
24	r	303	CHL	CHD-C4C-C3C	-5.21	117.18	124.84
24	8	303	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
24	1	304	CHL	O2D-CGD-CBD	5.21	120.53	111.27
31	C	615	8CT	C19-C20-C21	-5.21	119.87	127.31
24	N	310	CHL	CHB-C1B-NB	-5.21	118.74	124.26
24	7	312	CHL	C2A-C1A-CHA	-5.21	114.75	123.86
24	y	311	CHL	CHD-C4C-C3C	-5.21	117.19	124.84
24	G	313	CHL	O2D-CGD-CBD	5.21	120.52	111.27
24	p	305	CHL	O2D-CGD-CBD	5.21	120.52	111.27
24	n	312	CHL	C3B-C2B-C1B	-5.21	100.88	107.16
24	p	313	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
24	S	608	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
24	q	308	CHL	CHD-C4C-C3C	-5.20	117.19	124.84
24	G	306	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
24	6	311	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
24	g	313	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
24	g	312	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
24	N	311	CHL	CHD-C4C-C3C	-5.19	117.21	124.84
24	6	309	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
24	8	308	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
24	p	312	CHL	C2A-C1A-CHA	-5.19	114.78	123.86
24	n	311	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
31	D	410	8CT	C14-C13-C12	-5.19	119.91	127.31
24	7	318	CHL	CHB-C1B-NB	-5.19	118.77	124.26
24	2	306	CHL	CHD-C4C-C3C	-5.19	117.22	124.84
24	2	311	CHL	C3B-C2B-C1B	-5.19	100.90	107.16
24	Y	304	CHL	O2D-CGD-CBD	5.18	120.48	111.27
24	1	310	CHL	C3B-C2B-C1B	-5.18	100.90	107.16
24	9	309	CHL	C3B-C2B-C1B	-5.18	100.90	107.16
24	s	414	CHL	CHD-C4C-C3C	-5.18	117.22	124.84
24	G	309	CHL	C4A-NA-C1A	5.18	109.03	106.71
24	N	309	CHL	O2D-CGD-CBD	5.18	120.47	111.27
24	5	313	CHL	O2D-CGD-CBD	5.18	120.47	111.27
24	R	602	CHL	CHD-C4C-C3C	-5.18	117.23	124.84
24	8	308	CHL	CHD-C4C-C3C	-5.18	117.23	124.84
24	n	310	CHL	CHB-C1B-NB	-5.18	118.78	124.26
31	x	601	8CT	C01-C02-C03	-5.18	118.72	124.53
24	7	313	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
24	4	304	CHL	O2D-CGD-CBD	5.17	120.46	111.27
24	7	309	CHL	O2D-CGD-CBD	5.17	120.46	111.27
24	3	311	CHL	C3B-C2B-C1B	-5.17	100.92	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	311	CHL	CHB-C1B-NB	-5.17	118.78	124.26
24	2	313	CHL	O2D-CGD-CBD	5.17	120.46	111.27
24	8	308	CHL	C2A-C1A-CHA	-5.17	114.82	123.86
24	5	311	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
24	6	312	CHL	CHB-C1B-NB	-5.17	118.78	124.26
24	6	304	CHL	CHB-C1B-NB	-5.17	118.79	124.26
24	6	305	CHL	O2D-CGD-CBD	5.17	120.45	111.27
24	n	310	CHL	O2D-CGD-CBD	5.16	120.44	111.27
24	g	313	CHL	CHB-C1B-NB	-5.16	118.79	124.26
24	8	310	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
24	n	305	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
24	q	310	CHL	C2A-C1A-CHA	-5.16	114.84	123.86
24	g	306	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
24	3	312	CHL	CHB-C1B-NB	-5.16	118.80	124.26
24	Y	304	CHL	C3B-C2B-C1B	-5.16	100.94	107.16
24	g	311	CHL	C1D-ND-C4D	5.16	110.00	106.33
24	u	312	CHL	C1D-ND-C4D	5.16	110.00	106.33
24	u	306	CHL	C3B-C2B-C1B	-5.16	100.94	107.16
24	q	311	CHL	C3B-C2B-C1B	-5.16	100.94	107.16
24	1	309	CHL	C1D-ND-C4D	5.15	110.00	106.33
24	9	304	CHL	CHB-C1B-NB	-5.15	118.80	124.26
24	S	613	CHL	CHD-C4C-C3C	-5.15	117.27	124.84
24	G	313	CHL	C3B-C2B-C1B	-5.15	100.95	107.16
24	s	403	CHL	C3B-C2B-C1B	-5.15	100.95	107.16
31	c	615	8CT	C01-C02-C03	-5.15	118.75	124.53
24	5	310	CHL	CHD-C4C-C3C	-5.15	117.28	124.84
24	u	310	CHL	C3B-C2B-C1B	-5.14	100.95	107.16
24	y	305	CHL	C3B-C2B-C1B	-5.14	100.95	107.16
24	3	310	CHL	O2D-CGD-CBD	5.14	120.41	111.27
24	4	312	CHL	C1D-ND-C4D	5.14	109.99	106.33
24	p	309	CHL	O2D-CGD-CBD	5.14	120.40	111.27
24	S	602	CHL	C3B-C2B-C1B	-5.14	100.96	107.16
24	6	310	CHL	O2D-CGD-CBD	5.14	120.39	111.27
31	c	615	8CT	C19-C20-C21	-5.13	119.98	127.31
24	3	305	CHL	O2D-CGD-CBD	5.13	120.39	111.27
24	p	318	CHL	CHB-C1B-NB	-5.13	118.83	124.26
24	3	309	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
24	R	606	CHL	CHD-C4C-C3C	-5.13	117.31	124.84
24	1	305	CHL	CHD-C4C-C3C	-5.12	117.31	124.84
24	N	317	CHL	C4A-NA-C1A	5.12	109.01	106.71
24	g	313	CHL	O2D-CGD-CBD	5.12	120.37	111.27
24	9	317	CHL	O2D-CGD-CBD	5.12	120.36	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	409	CHL	C3B-C2B-C1B	-5.12	100.98	107.16
28	2	304	NEX	C15-C35-C34	5.12	133.96	123.47
28	9	319	NEX	C15-C35-C34	5.12	133.95	123.47
28	5	304	NEX	C15-C35-C34	5.12	133.95	123.47
24	N	310	CHL	O2D-CGD-CBD	5.12	120.36	111.27
24	G	318	CHL	O2D-CGD-CBD	5.11	120.36	111.27
24	5	313	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
24	N	305	CHL	CHD-C4C-C3C	-5.11	117.32	124.84
28	p	304	NEX	C15-C35-C34	5.11	133.95	123.47
24	n	305	CHL	CHD-C4C-C3C	-5.11	117.32	124.84
24	S	601	CHL	CHD-C4C-C3C	-5.11	117.32	124.84
24	S	607	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
24	n	317	CHL	C4A-NA-C1A	5.11	109.00	106.71
24	y	309	CHL	CHB-C1B-NB	-5.11	118.85	124.26
24	1	312	CHL	C1D-ND-C4D	5.11	109.96	106.33
24	N	310	CHL	C1D-ND-C4D	5.11	109.96	106.33
24	2	310	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
24	y	310	CHL	C3B-C2B-C1B	-5.10	101.00	107.16
24	5	312	CHL	CHD-C4C-C3C	-5.10	117.34	124.84
24	9	311	CHL	C1D-ND-C4D	5.10	109.96	106.33
24	u	310	CHL	CHB-C1B-NB	-5.10	118.86	124.26
24	4	309	CHL	C1D-ND-C4D	5.10	109.96	106.33
24	n	310	CHL	C1D-ND-C4D	5.10	109.96	106.33
28	S	617	NEX	C15-C35-C34	5.10	133.91	123.47
24	u	310	CHL	C1D-ND-C4D	5.09	109.95	106.33
24	n	309	CHL	O2D-CGD-CBD	5.09	120.32	111.27
24	9	308	CHL	O2D-CGD-CBD	5.09	120.32	111.27
24	R	608	CHL	O2D-CGD-CBD	5.09	120.31	111.27
28	R	616	NEX	C15-C35-C34	5.09	133.89	123.47
24	q	307	CHL	CHB-C1B-NB	-5.09	118.87	124.26
24	p	318	CHL	O2D-CGD-CBD	5.09	120.31	111.27
28	1	303	NEX	C15-C35-C34	5.09	133.89	123.47
28	g	304	NEX	C15-C35-C34	5.08	133.89	123.47
24	N	305	CHL	O2D-CGD-CBD	5.08	120.30	111.27
24	4	308	CHL	O2D-CGD-CBD	5.08	120.30	111.27
24	2	313	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
31	X	601	8CT	C01-C02-C03	-5.08	118.82	124.53
24	1	309	CHL	O2D-CGD-CBD	5.08	120.30	111.27
24	S	608	CHL	O2D-CGD-CBD	5.08	120.30	111.27
29	2	301	0UR	C10-C11-C12	-5.08	120.06	127.31
28	u	304	NEX	C15-C35-C34	5.08	133.88	123.47
24	Y	319	CHL	O2D-CGD-CBD	5.08	120.29	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	305	CHL	CHD-C4C-C3C	-5.08	117.38	124.84
28	4	303	NEX	C15-C35-C34	5.08	133.87	123.47
24	y	318	CHL	O2D-CGD-CBD	5.08	120.29	111.27
28	r	317	NEX	C15-C35-C34	5.08	133.87	123.47
24	S	602	CHL	O2D-CGD-CBD	5.07	120.28	111.27
29	5	301	0UR	C10-C11-C12	-5.07	120.07	127.31
24	Y	317	CHL	O2D-CGD-CBD	5.07	120.28	111.27
24	9	305	CHL	O2D-CGD-CBD	5.07	120.28	111.27
28	7	304	NEX	C15-C35-C34	5.07	133.85	123.47
24	s	403	CHL	O2D-CGD-CBD	5.07	120.27	111.27
24	4	310	CHL	O2D-CGD-CBD	5.07	120.27	111.27
24	2	312	CHL	CHD-C4C-C3C	-5.07	117.39	124.84
24	7	318	CHL	O2D-CGD-CBD	5.06	120.27	111.27
24	Y	309	CHL	C3B-C2B-C1B	-5.06	101.05	107.16
24	3	312	CHL	O2D-CGD-CBD	5.06	120.27	111.27
24	g	318	CHL	O2D-CGD-CBD	5.06	120.27	111.27
24	u	310	CHL	O2D-CGD-CBD	5.06	120.26	111.27
24	s	409	CHL	O2D-CGD-CBD	5.06	120.26	111.27
24	6	317	CHL	C1D-ND-C4D	5.06	109.93	106.33
24	u	309	CHL	O2D-CGD-CBD	5.06	120.26	111.27
24	6	311	CHL	CHD-C4C-C3C	-5.06	117.40	124.84
24	u	318	CHL	O2D-CGD-CBD	5.06	120.26	111.27
24	1	308	CHL	O2D-CGD-CBD	5.06	120.25	111.27
24	8	303	CHL	O2D-CGD-CBD	5.06	120.25	111.27
24	4	309	CHL	C3B-C2B-C1B	-5.06	101.06	107.16
28	G	304	NEX	C15-C35-C34	5.05	133.83	123.47
28	y	304	NEX	C15-C35-C34	5.05	133.83	123.47
24	4	309	CHL	O2D-CGD-CBD	5.05	120.25	111.27
24	y	305	CHL	O2D-CGD-CBD	5.05	120.25	111.27
24	9	305	CHL	C3B-C2B-C1B	-5.05	101.06	107.16
24	g	309	CHL	C4A-NA-C1A	5.05	108.98	106.71
31	T	101	8CT	C19-C20-C21	-5.05	120.11	127.31
24	Y	312	CHL	C3B-C2B-C1B	-5.04	101.08	107.16
24	r	309	CHL	O2D-CGD-CBD	5.04	120.23	111.27
31	t	101	8CT	C19-C20-C21	-5.04	120.12	127.31
24	y	311	CHL	C2A-C1A-CHA	-5.04	115.05	123.86
24	R	605	CHL	O2D-CGD-CBD	5.04	120.22	111.27
24	1	309	CHL	C3B-C2B-C1B	-5.04	101.08	107.16
24	q	316	CHL	O2D-CGD-CBD	5.04	120.22	111.27
31	C	615	8CT	C14-C13-C12	-5.04	120.12	127.31
24	y	306	CHL	O2D-CGD-CBD	5.04	120.22	111.27
24	6	312	CHL	O2D-CGD-CBD	5.04	120.22	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	319	CHL	CHD-C4C-C3C	-5.04	117.44	124.84
24	g	306	CHL	CHD-C4C-C3C	-5.03	117.44	124.84
24	S	602	CHL	C2A-C1A-CHA	-5.03	115.06	123.86
24	Y	305	CHL	O2D-CGD-CBD	5.03	120.21	111.27
24	7	310	CHL	O2D-CGD-CBD	5.03	120.21	111.27
24	1	310	CHL	O2D-CGD-CBD	5.03	120.20	111.27
24	8	315	CHL	O2D-CGD-CBD	5.03	120.20	111.27
24	q	307	CHL	C1D-ND-C4D	5.03	109.91	106.33
24	y	309	CHL	C1D-ND-C4D	5.03	109.91	106.33
24	q	307	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	3	309	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	g	310	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	G	311	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	6	304	CHL	C1D-ND-C4D	5.02	109.90	106.33
24	9	309	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	S	608	CHL	C2A-C1A-CHA	-5.02	115.09	123.86
24	s	402	CHL	CHD-C4C-C3C	-5.02	117.47	124.84
24	u	311	CHL	O2D-CGD-CBD	5.02	120.18	111.27
28	3	318	NEX	C27-C28-C29	-5.01	117.75	125.53
24	p	310	CHL	O2D-CGD-CBD	5.01	120.17	111.27
24	8	304	CHL	O2D-CGD-CBD	5.01	120.17	111.27
24	q	309	CHL	O2D-CGD-CBD	5.01	120.17	111.27
24	6	309	CHL	O2D-CGD-CBD	5.01	120.17	111.27
24	2	311	CHL	O2D-CGD-CBD	5.00	120.16	111.27
24	2	318	CHL	O2D-CGD-CBD	5.00	120.16	111.27
24	Y	308	CHL	C1D-ND-C4D	5.00	109.89	106.33
28	s	401	NEX	C27-C28-C29	-5.00	117.77	125.53
24	r	306	CHL	O2D-CGD-CBD	5.00	120.15	111.27
24	3	317	CHL	C1D-ND-C4D	4.99	109.88	106.33
28	6	303	NEX	C27-C28-C29	-4.99	117.78	125.53
31	D	410	8CT	C10-C11-C12	-4.99	118.69	126.23
24	n	317	CHL	O2D-CGD-CBD	4.99	120.13	111.27
24	G	309	CHL	O2D-CGD-CBD	4.99	120.13	111.27
24	y	313	CHL	C3B-C2B-C1B	-4.99	101.14	107.16
24	5	311	CHL	O2D-CGD-CBD	4.99	120.13	111.27
31	a	608	8CT	C01-C02-C03	-4.98	118.93	124.53
24	5	318	CHL	O2D-CGD-CBD	4.98	120.12	111.27
24	q	304	CHL	C2A-C1A-CHA	-4.98	115.15	123.86
28	r	301	NEX	C27-C28-C29	-4.98	117.80	125.53
24	q	303	CHL	O2D-CGD-CBD	4.98	120.12	111.27
24	u	306	CHL	O2D-CGD-CBD	4.98	120.12	111.27
24	G	310	CHL	C1D-ND-C4D	4.98	109.87	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	310	CHL	C1D-ND-C4D	4.98	109.87	106.33
31	A	608	8CT	C01-C02-C03	-4.97	118.94	124.53
28	N	303	NEX	C27-C28-C29	-4.97	117.81	125.53
24	G	306	CHL	O2D-CGD-CBD	4.97	120.10	111.27
28	n	303	NEX	C27-C28-C29	-4.97	117.82	125.53
24	q	304	CHL	O2D-CGD-CBD	4.97	120.10	111.27
26	9	303	0IE	C20-C3-C4	-4.97	118.44	124.83
24	p	309	CHL	C4A-NA-C1A	4.97	108.94	106.71
28	6	303	NEX	C35-C34-C33	-4.96	120.22	127.31
24	q	309	CHL	CHD-C4C-C3C	-4.96	117.54	124.84
24	r	307	CHL	CHD-C4C-C3C	-4.96	117.54	124.84
28	N	303	NEX	C35-C34-C33	-4.96	120.23	127.31
24	9	310	CHL	O2D-CGD-CBD	4.96	120.08	111.27
24	N	317	CHL	O2D-CGD-CBD	4.96	120.08	111.27
24	Y	310	CHL	C2A-C1A-CHA	-4.95	115.20	123.86
24	N	308	CHL	O2D-CGD-CBD	4.95	120.07	111.27
24	G	313	CHL	CHB-C1B-NB	-4.95	119.02	124.26
28	r	301	NEX	C35-C34-C33	-4.95	120.25	127.31
24	g	309	CHL	O2D-CGD-CBD	4.95	120.06	111.27
24	N	308	CHL	C1D-ND-C4D	4.95	109.85	106.33
24	3	309	CHL	CHB-C1B-NB	-4.94	119.02	124.26
24	g	306	CHL	O2D-CGD-CBD	4.94	120.05	111.27
24	9	309	CHL	CHB-C1B-NB	-4.94	119.03	124.26
24	S	601	CHL	O2D-CGD-CBD	4.94	120.05	111.27
24	4	311	CHL	C3B-C2B-C1B	-4.93	101.21	107.16
31	s	415	8CT	C19-C20-C21	-4.93	120.27	127.31
24	y	311	CHL	O2D-CGD-CBD	4.93	120.03	111.27
24	7	310	CHL	C1D-ND-C4D	4.93	109.84	106.33
24	3	311	CHL	CHD-C4C-C3C	-4.92	117.60	124.84
24	G	311	CHL	C1D-ND-C4D	4.92	109.83	106.33
28	3	318	NEX	C35-C34-C33	-4.92	120.28	127.31
28	s	401	NEX	C35-C34-C33	-4.92	120.28	127.31
24	G	310	CHL	O2D-CGD-CBD	4.92	120.01	111.27
24	q	311	CHL	C2A-C1A-CHA	-4.92	115.25	123.86
24	2	311	CHL	C1D-ND-C4D	4.92	109.83	106.33
24	1	311	CHL	C3B-C2B-C1B	-4.92	101.22	107.16
24	Y	305	CHL	C2A-C1A-CHA	-4.91	115.27	123.86
24	y	306	CHL	C2A-C1A-CHA	-4.91	115.27	123.86
24	5	311	CHL	C1D-ND-C4D	4.91	109.83	106.33
24	p	310	CHL	C1D-ND-C4D	4.91	109.83	106.33
24	8	307	CHL	C1D-ND-C4D	4.91	109.82	106.33
31	d	410	8CT	C10-C11-C12	-4.91	118.82	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	309	CHL	CHB-C1B-NB	-4.90	119.06	124.26
24	s	403	CHL	C2A-C1A-CHA	-4.90	115.28	123.86
24	p	311	CHL	O2D-CGD-CBD	4.90	119.98	111.27
24	G	306	CHL	C2A-C1A-CHA	-4.90	115.28	123.86
24	s	402	CHL	O2D-CGD-CBD	4.90	119.98	111.27
24	2	306	CHL	O2D-CGD-CBD	4.90	119.97	111.27
24	R	602	CHL	C2A-C1A-CHA	-4.90	115.29	123.86
24	g	310	CHL	CHB-C1B-NB	-4.90	119.07	124.26
24	S	605	CHL	O2D-CGD-CBD	4.90	119.97	111.27
24	8	310	CHL	O2D-CGD-CBD	4.90	119.97	111.27
24	u	305	CHL	O2D-CGD-CBD	4.89	119.97	111.27
28	n	303	NEX	C35-C34-C33	-4.89	120.33	127.31
24	7	313	CHL	O2D-CGD-CBD	4.89	119.96	111.27
24	5	306	CHL	O2D-CGD-CBD	4.89	119.96	111.27
24	r	303	CHL	C2A-C1A-CHA	-4.89	115.31	123.86
24	8	307	CHL	CHB-C1B-NB	-4.89	119.08	124.26
24	1	311	CHL	C2A-C1A-CHA	-4.89	115.32	123.86
24	q	304	CHL	CHD-C4C-C3C	-4.89	117.66	124.84
29	u	301	0UR	C9-C8-C7	-4.89	120.34	127.31
24	9	304	CHL	O2D-CGD-CBD	4.88	119.95	111.27
24	q	304	CHL	C3B-C2B-C1B	-4.88	101.27	107.16
24	7	318	CHL	C1D-ND-C4D	4.87	109.80	106.33
31	S	614	8CT	C19-C20-C21	-4.87	120.36	127.31
24	p	313	CHL	O2D-CGD-CBD	4.87	119.93	111.27
24	s	406	CHL	O2D-CGD-CBD	4.87	119.92	111.27
24	9	309	CHL	C1D-ND-C4D	4.87	109.79	106.33
24	3	308	CHL	O2D-CGD-CBD	4.87	119.92	111.27
24	8	304	CHL	CHD-C4C-C3C	-4.86	117.69	124.84
24	6	308	CHL	O2D-CGD-CBD	4.86	119.90	111.27
24	6	305	CHL	CHD-C4C-C3C	-4.86	117.70	124.84
24	6	304	CHL	O2D-CGD-CBD	4.86	119.90	111.27
24	G	310	CHL	CHB-C1B-NB	-4.85	119.12	124.26
24	q	311	CHL	O2D-CGD-CBD	4.85	119.89	111.27
24	u	313	CHL	O2D-CGD-CBD	4.85	119.89	111.27
24	Y	310	CHL	O2D-CGD-CBD	4.85	119.89	111.27
24	p	318	CHL	C1D-ND-C4D	4.85	109.78	106.33
24	8	309	CHL	C3B-C2B-C1B	-4.85	101.31	107.16
24	s	409	CHL	C2A-C1A-CHA	-4.85	115.38	123.86
28	4	303	NEX	C15-C14-C13	-4.85	120.39	127.31
24	9	312	CHL	O2D-CGD-CBD	4.84	119.88	111.27
24	8	310	CHL	C2A-C1A-CHA	-4.84	115.39	123.86
24	2	310	CHL	O2D-CGD-CBD	4.84	119.87	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	u	306	CHL	CHD-C4C-C3C	-4.84	117.73	124.84
24	8	304	CHL	C3B-C2B-C1B	-4.84	101.32	107.16
24	G	312	CHL	CHB-C1B-NB	-4.84	119.13	124.26
28	2	304	NEX	C15-C14-C13	-4.84	120.40	127.31
24	S	606	CHL	O2D-CGD-CBD	4.84	119.86	111.27
29	N	301	0UR	C10-C11-C12	-4.84	120.41	127.31
24	G	306	CHL	CHD-C4C-C3C	-4.84	117.73	124.84
24	r	309	CHL	CHD-C4C-C3C	-4.84	117.73	124.84
28	y	304	NEX	C15-C14-C13	-4.83	120.41	127.31
39	D	406	PL9	C7-C3-C4	4.83	120.80	116.88
28	G	304	NEX	C15-C14-C13	-4.83	120.42	127.31
24	1	311	CHL	CHD-C4C-C3C	-4.82	117.75	124.84
24	2	313	CHL	C1D-ND-C4D	4.82	109.76	106.33
24	R	607	CHL	C2A-C1A-CHA	-4.82	115.43	123.86
24	1	312	CHL	CHB-C1B-NB	-4.82	119.15	124.26
24	4	310	CHL	CHB-C1B-NB	-4.82	119.15	124.26
24	4	312	CHL	CHB-C1B-NB	-4.82	119.15	124.26
31	V	401	8CT	C18-C17-C16	-4.82	120.43	127.31
24	9	308	CHL	C4A-NA-C1A	4.82	108.87	106.71
24	8	304	CHL	C2A-C1A-CHA	-4.82	115.44	123.86
24	5	310	CHL	O2D-CGD-CBD	4.82	119.83	111.27
28	9	319	NEX	C15-C14-C13	-4.81	120.44	127.31
31	B	617	8CT	C24-C25-C26	-4.81	120.44	127.31
24	s	407	CHL	O2D-CGD-CBD	4.81	119.82	111.27
28	S	617	NEX	C15-C14-C13	-4.81	120.44	127.31
24	G	305	CHL	CHB-C1B-NB	-4.81	119.16	124.26
24	y	309	CHL	O2D-CGD-CBD	4.81	119.82	111.27
28	R	616	NEX	C15-C14-C13	-4.81	120.44	127.31
24	q	310	CHL	C3B-C2B-C1B	-4.81	101.35	107.16
29	n	301	0UR	C10-C11-C12	-4.81	120.44	127.31
24	N	308	CHL	CHB-C1B-NB	-4.81	119.17	124.26
24	9	305	CHL	CHD-C4C-C3C	-4.81	117.77	124.84
24	Y	309	CHL	O2D-CGD-CBD	4.81	119.81	111.27
24	Y	308	CHL	O2D-CGD-CBD	4.81	119.81	111.27
24	Y	312	CHL	C2A-C1A-CHA	-4.81	115.45	123.86
28	5	304	NEX	C15-C14-C13	-4.81	120.45	127.31
28	7	304	NEX	C15-C14-C13	-4.81	120.45	127.31
24	4	311	CHL	O2D-CGD-CBD	4.80	119.81	111.27
24	y	310	CHL	O2D-CGD-CBD	4.80	119.80	111.27
28	p	304	NEX	C15-C14-C13	-4.80	120.46	127.31
28	r	317	NEX	C15-C14-C13	-4.80	120.46	127.31
24	9	304	CHL	C1D-ND-C4D	4.80	109.75	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	305	CHL	O2D-CGD-CBD	4.80	119.80	111.27
31	C	614	8CT	C07-C02-C03	-4.80	115.76	122.73
24	y	312	CHL	C2A-C1A-CHA	-4.80	115.47	123.86
33	W	201	LMG	O7-C10-C11	4.80	121.84	111.50
24	7	311	CHL	CHD-C4C-C3C	-4.80	117.79	124.84
24	3	309	CHL	C1D-ND-C4D	4.80	109.74	106.33
24	5	313	CHL	C1D-ND-C4D	4.80	109.74	106.33
24	g	305	CHL	CHB-C1B-NB	-4.79	119.18	124.26
24	Y	311	CHL	C2A-C1A-CHA	-4.79	115.48	123.86
24	G	318	CHL	CHD-C4C-C3C	-4.79	117.80	124.84
28	1	303	NEX	C15-C14-C13	-4.79	120.47	127.31
39	d	406	PL9	C7-C3-C4	4.79	120.77	116.88
24	G	305	CHL	C1D-ND-C4D	4.78	109.73	106.33
24	2	313	CHL	CHB-C1B-NB	-4.78	119.20	124.26
28	u	304	NEX	C15-C14-C13	-4.78	120.49	127.31
28	g	304	NEX	C15-C14-C13	-4.78	120.49	127.31
24	2	305	CHL	O2D-CGD-CBD	4.77	119.75	111.27
24	1	310	CHL	CHB-C1B-NB	-4.77	119.20	124.26
24	3	304	CHL	O2D-CGD-CBD	4.77	119.75	111.27
24	g	305	CHL	C1D-ND-C4D	4.77	109.72	106.33
24	r	308	CHL	C2A-C1A-CHA	-4.77	115.52	123.86
24	6	309	CHL	C1D-ND-C4D	4.77	109.72	106.33
24	9	317	CHL	C4A-NA-C1A	4.77	108.85	106.71
24	3	305	CHL	CHD-C4C-C3C	-4.77	117.83	124.84
31	c	615	8CT	C14-C13-C12	-4.77	120.51	127.31
28	r	301	NEX	O24-C25-C38	4.76	120.76	115.06
28	N	303	NEX	O24-C25-C38	4.76	120.76	115.06
24	R	608	CHL	CHD-C4C-C3C	-4.76	117.85	124.84
28	n	303	NEX	O24-C25-C38	4.76	120.75	115.06
24	G	305	CHL	O2D-CGD-CBD	4.76	119.72	111.27
24	1	311	CHL	O2D-CGD-CBD	4.75	119.72	111.27
33	w	201	LMG	O7-C10-C11	4.75	121.75	111.50
24	2	311	CHL	CHB-C1B-NB	-4.75	119.23	124.26
29	G	301	0UR	C10-C11-C12	-4.75	120.53	127.31
28	3	318	NEX	O24-C25-C38	4.75	120.75	115.06
24	g	318	CHL	CHD-C4C-C3C	-4.74	117.87	124.84
24	g	305	CHL	O2D-CGD-CBD	4.74	119.70	111.27
24	5	313	CHL	CHB-C1B-NB	-4.74	119.24	124.26
24	2	305	CHL	CHB-C1B-NB	-4.73	119.25	124.26
31	c	614	8CT	C07-C02-C03	-4.73	115.86	122.73
29	u	301	0UR	C10-C11-C12	-4.73	120.56	127.31
24	1	310	CHL	CHD-C4C-C3C	-4.73	117.89	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	605	CHL	C1D-ND-C4D	4.73	109.69	106.33
24	5	311	CHL	CHB-C1B-NB	-4.73	119.25	124.26
31	S	615	8CT	C30-C31-C32	-4.73	115.65	121.47
28	s	401	NEX	O24-C25-C38	4.72	120.72	115.06
28	6	303	NEX	O24-C25-C38	4.72	120.71	115.06
31	C	613	8CT	C35-C30-C29	-4.72	106.73	112.70
24	3	304	CHL	CHB-C1B-NB	-4.72	119.26	124.26
24	n	312	CHL	C2A-C1A-CHA	-4.72	115.61	123.86
24	4	311	CHL	CHD-C4C-C3C	-4.72	117.91	124.84
31	C	614	8CT	C10-C11-C12	-4.71	119.11	126.23
31	c	614	8CT	C10-C11-C12	-4.71	119.11	126.23
24	N	312	CHL	C2A-C1A-CHA	-4.71	115.62	123.86
24	s	407	CHL	CHD-C4C-C3C	-4.71	117.92	124.84
24	n	308	CHL	O2D-CGD-CBD	4.71	119.63	111.27
24	s	406	CHL	C1D-ND-C4D	4.71	109.68	106.33
24	1	317	CHL	C4A-NA-C1A	4.70	108.82	106.71
24	p	310	CHL	CHB-C1B-NB	-4.70	119.29	124.26
24	S	606	CHL	CHD-C4C-C3C	-4.69	117.94	124.84
24	r	306	CHL	CHB-C1B-NB	-4.69	119.29	124.26
24	4	310	CHL	CHD-C4C-C3C	-4.69	117.95	124.84
24	1	310	CHL	C1D-ND-C4D	4.69	109.66	106.33
24	4	311	CHL	C2A-C1A-CHA	-4.68	115.67	123.86
31	b	617	8CT	C24-C25-C26	-4.68	120.63	127.31
24	4	310	CHL	C1D-ND-C4D	4.68	109.66	106.33
24	5	306	CHL	C2A-C1A-CHA	-4.68	115.68	123.86
29	9	301	0UR	C10-C11-C12	-4.68	120.64	127.31
24	s	406	CHL	CHD-C4C-C3C	-4.67	117.97	124.84
31	s	416	8CT	C30-C31-C32	-4.67	115.72	121.47
24	p	311	CHL	CHD-C4C-C3C	-4.67	117.97	124.84
28	9	319	NEX	C31-C30-C29	-4.67	120.64	127.31
28	u	304	NEX	C31-C30-C29	-4.67	120.64	127.31
24	5	312	CHL	C2A-C1A-CHA	-4.67	115.69	123.86
24	7	310	CHL	CHB-C1B-NB	-4.67	119.31	124.26
26	3	303	0IE	C20-C3-C4	-4.67	118.82	124.83
24	S	605	CHL	CHD-C4C-C3C	-4.67	117.98	124.84
24	S	608	CHL	CHD-C4C-C3C	-4.67	117.98	124.84
24	2	309	CHL	O2D-CGD-CBD	4.67	119.56	111.27
28	5	304	NEX	C31-C30-C29	-4.67	120.65	127.31
28	p	304	NEX	C31-C30-C29	-4.67	120.65	127.31
24	g	318	CHL	C1D-ND-C4D	4.67	109.65	106.33
29	g	301	0UR	C10-C11-C12	-4.67	120.65	127.31
24	5	305	CHL	CHD-C4C-C3C	-4.66	117.98	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	306	CHL	C1D-ND-C4D	4.66	109.65	106.33
24	n	304	CHL	O2D-CGD-CBD	4.66	119.55	111.27
24	R	608	CHL	C2A-C1A-CHA	-4.66	115.72	123.86
24	9	311	CHL	CHD-C4C-C3C	-4.66	118.00	124.84
24	G	312	CHL	C1D-ND-C4D	4.66	109.64	106.33
24	n	311	CHL	C2A-C1A-CHA	-4.65	115.72	123.86
24	N	304	CHL	O2D-CGD-CBD	4.65	119.53	111.27
24	Y	312	CHL	CHD-C4C-C3C	-4.65	118.00	124.84
31	v	401	8CT	C18-C17-C16	-4.65	120.67	127.31
24	2	306	CHL	C2A-C1A-CHA	-4.65	115.73	123.86
24	2	305	CHL	C1D-ND-C4D	4.65	109.64	106.33
24	7	313	CHL	C2A-C1A-CHA	-4.65	115.73	123.86
28	7	304	NEX	C31-C30-C29	-4.65	120.68	127.31
24	r	309	CHL	C2A-C1A-CHA	-4.65	115.73	123.86
24	r	306	CHL	CHD-C4C-C3C	-4.65	118.01	124.84
28	y	304	NEX	C31-C30-C29	-4.65	120.68	127.31
24	u	318	CHL	C4A-NA-C1A	4.65	108.80	106.71
24	2	305	CHL	CHD-C4C-C3C	-4.65	118.01	124.84
24	g	305	CHL	CHD-C4C-C3C	-4.64	118.01	124.84
24	S	607	CHL	O2D-CGD-CBD	4.64	119.52	111.27
28	S	617	NEX	C31-C30-C29	-4.64	120.68	127.31
28	r	317	NEX	C38-C25-C24	-4.64	109.06	114.28
29	6	301	0UR	C10-C11-C12	-4.64	120.68	127.31
28	4	303	NEX	C31-C30-C29	-4.64	120.69	127.31
31	C	613	8CT	C24-C25-C26	-4.63	120.70	127.31
28	g	304	NEX	O24-C25-C38	4.63	120.61	115.06
24	S	606	CHL	CHB-C1B-NB	-4.63	119.35	124.26
28	G	304	NEX	C31-C30-C29	-4.63	120.70	127.31
28	g	304	NEX	C38-C25-C24	-4.63	109.07	114.28
24	p	313	CHL	C2A-C1A-CHA	-4.63	115.77	123.86
28	R	616	NEX	C31-C30-C29	-4.63	120.71	127.31
24	y	313	CHL	O2D-CGD-CBD	4.63	119.49	111.27
24	q	310	CHL	O2D-CGD-CBD	4.63	119.49	111.27
28	1	303	NEX	C31-C30-C29	-4.63	120.71	127.31
24	y	318	CHL	C2A-C1A-CHA	-4.62	115.78	123.85
24	y	313	CHL	C2A-C1A-CHA	-4.62	115.78	123.86
24	G	305	CHL	CHD-C4C-C3C	-4.62	118.05	124.84
28	r	317	NEX	C31-C30-C29	-4.62	120.71	127.31
28	2	304	NEX	C31-C30-C29	-4.62	120.72	127.31
28	1	303	NEX	C38-C25-C24	-4.62	109.08	114.28
24	8	309	CHL	O2D-CGD-CBD	4.62	119.47	111.27
28	r	317	NEX	O24-C25-C38	4.61	120.58	115.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	312	CHL	CHB-C1B-NB	-4.61	119.37	124.26
24	S	606	CHL	C1D-ND-C4D	4.61	109.61	106.33
24	1	317	CHL	O2D-CGD-CBD	4.61	119.46	111.27
24	s	406	CHL	CHB-C1B-NB	-4.61	119.38	124.26
24	Y	317	CHL	C2A-C1A-CHA	-4.61	115.81	123.85
24	q	316	CHL	C4A-NA-C1A	4.61	108.78	106.71
24	4	317	CHL	O2D-CGD-CBD	4.61	119.45	111.27
28	R	616	NEX	O24-C25-C38	4.61	120.58	115.06
28	R	616	NEX	C38-C25-C24	-4.61	109.10	114.28
24	y	313	CHL	C1D-ND-C4D	4.61	109.61	106.33
28	g	304	NEX	C31-C30-C29	-4.61	120.74	127.31
24	p	318	CHL	CHD-C4C-C3C	-4.61	118.07	124.84
24	7	311	CHL	CHB-C1B-NB	-4.60	119.38	124.26
28	y	304	NEX	O24-C25-C38	4.60	120.57	115.06
28	4	303	NEX	C38-C25-C24	-4.60	109.10	114.28
24	3	304	CHL	C1D-ND-C4D	4.60	109.61	106.33
24	s	407	CHL	C1D-ND-C4D	4.60	109.61	106.33
24	9	305	CHL	C2A-C1A-CHA	-4.60	115.81	123.86
24	s	407	CHL	CHB-C1B-NB	-4.60	119.39	124.26
24	s	409	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
28	G	304	NEX	C38-C25-C24	-4.60	109.11	114.28
24	q	311	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
24	N	305	CHL	C2A-C1A-CHA	-4.60	115.82	123.86
24	Y	319	CHL	C2A-C1A-CHA	-4.60	115.82	123.86
28	y	304	NEX	C38-C25-C24	-4.60	109.11	114.28
28	p	304	NEX	C38-C25-C24	-4.60	109.11	114.28
24	p	311	CHL	CHB-C1B-NB	-4.60	119.39	124.26
28	1	303	NEX	O24-C25-C38	4.60	120.56	115.06
24	1	304	CHL	C4A-NA-C1A	4.60	108.77	106.71
24	7	318	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
24	Y	312	CHL	O2D-CGD-CBD	4.60	119.44	111.27
28	7	304	NEX	O24-C25-C38	4.59	120.56	115.06
28	4	303	NEX	O24-C25-C38	4.59	120.56	115.06
24	4	304	CHL	C4A-NA-C1A	4.59	108.77	106.71
24	5	309	CHL	O2D-CGD-CBD	4.59	119.42	111.27
24	u	312	CHL	CHD-C4C-C3C	-4.59	118.09	124.84
24	2	312	CHL	C2A-C1A-CHA	-4.59	115.83	123.86
24	G	318	CHL	C1D-ND-C4D	4.59	109.59	106.33
28	p	304	NEX	O24-C25-C38	4.59	120.55	115.06
24	7	313	CHL	C1D-ND-C4D	4.58	109.59	106.33
24	g	311	CHL	O2D-CGD-CBD	4.58	119.41	111.27
28	7	304	NEX	C38-C25-C24	-4.58	109.13	114.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	310	CHL	CHD-C4C-C3C	-4.58	118.11	124.84
24	p	313	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
28	5	304	NEX	O24-C25-C38	4.57	120.54	115.06
28	S	617	NEX	O24-C25-C38	4.57	120.53	115.06
24	7	313	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
24	g	312	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
24	5	305	CHL	CHB-C1B-NB	-4.57	119.42	124.26
28	5	304	NEX	C38-C25-C24	-4.56	109.14	114.28
24	S	605	CHL	CHB-C1B-NB	-4.56	119.43	124.26
24	u	309	CHL	C4A-NA-C1A	4.56	108.76	106.71
24	7	311	CHL	C1D-ND-C4D	4.56	109.57	106.33
28	9	319	NEX	O24-C25-C38	4.56	120.52	115.06
24	u	306	CHL	C2A-C1A-CHA	-4.56	115.89	123.86
24	4	317	CHL	C4A-NA-C1A	4.55	108.75	106.71
24	8	307	CHL	CHD-C4C-C3C	-4.55	118.15	124.84
28	S	617	NEX	C38-C25-C24	-4.55	109.16	114.28
31	c	613	8CT	C24-C25-C26	-4.55	120.82	127.31
31	c	615	8CT	C18-C17-C16	-4.55	120.82	127.31
29	8	301	0UR	C10-C11-C12	-4.55	120.82	127.31
24	g	318	CHL	CHB-C1B-NB	-4.55	119.44	124.26
24	y	313	CHL	CHD-C4C-C3C	-4.55	118.16	124.84
28	u	304	NEX	C38-C25-C24	-4.54	109.17	114.28
24	R	606	CHL	C2A-C1A-CHA	-4.54	115.91	123.86
28	u	304	NEX	O24-C25-C38	4.54	120.50	115.06
31	c	613	8CT	C35-C30-C29	-4.54	106.96	112.70
28	G	304	NEX	O24-C25-C38	4.54	120.49	115.06
24	u	312	CHL	O2D-CGD-CBD	4.54	119.33	111.27
28	2	304	NEX	C38-C25-C24	-4.54	109.18	114.28
28	9	319	NEX	C38-C25-C24	-4.54	109.18	114.28
24	p	311	CHL	C1D-ND-C4D	4.54	109.56	106.33
28	2	304	NEX	O24-C25-C38	4.53	120.49	115.06
24	2	312	CHL	O2D-CGD-CBD	4.53	119.32	111.27
24	s	408	CHL	O2D-CGD-CBD	4.52	119.30	111.27
24	r	307	CHL	CHB-C1B-NB	-4.52	119.47	124.26
24	n	305	CHL	C2A-C1A-CHA	-4.52	115.96	123.86
31	c	614	8CT	C01-C02-C03	-4.51	119.46	124.53
24	r	309	CHL	C1D-ND-C4D	4.51	109.54	106.33
24	3	311	CHL	O2D-CGD-CBD	4.51	119.28	111.27
26	3	303	0IE	C10-C9-C8	4.51	132.71	123.47
24	5	305	CHL	C1D-ND-C4D	4.51	109.54	106.33
24	1	309	CHL	CHB-C1B-NB	-4.50	119.49	124.26
31	C	614	8CT	C01-C02-C03	-4.50	119.47	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	311	CHL	O2D-CGD-CBD	4.50	119.27	111.27
24	6	305	CHL	C2A-C1A-CHA	-4.50	115.99	123.86
24	S	613	CHL	C2A-C1A-CHA	-4.50	115.99	123.85
24	8	315	CHL	C4A-NA-C1A	4.50	108.73	106.71
24	9	311	CHL	O2D-CGD-CBD	4.50	119.26	111.27
24	Y	312	CHL	C1D-ND-C4D	4.50	109.53	106.33
24	5	312	CHL	O2D-CGD-CBD	4.50	119.26	111.27
24	3	304	CHL	CHD-C4C-C3C	-4.50	118.23	124.84
24	1	305	CHL	C2A-C1A-CHA	-4.50	116.00	123.86
24	q	309	CHL	C2A-C1A-CHA	-4.50	116.00	123.86
24	p	313	CHL	C1D-ND-C4D	4.50	109.53	106.33
24	n	312	CHL	CHD-C4C-C3C	-4.50	118.23	124.84
31	d	410	8CT	C18-C17-C16	-4.49	120.89	127.31
24	g	312	CHL	C1D-ND-C4D	4.49	109.53	106.33
24	s	402	CHL	C1D-ND-C4D	4.49	109.53	106.33
30	Y	318	LHG	O7-C7-C8	4.49	121.18	111.50
24	n	311	CHL	O2D-CGD-CBD	4.49	119.25	111.27
33	B	619	LMG	O7-C10-C11	4.49	121.18	111.50
24	6	311	CHL	C2A-C1A-CHA	-4.49	116.01	123.86
24	3	311	CHL	CHB-C1B-NB	-4.49	119.51	124.26
30	d	408	LHG	O7-C7-C8	4.49	121.17	111.50
29	9	301	0UR	C9-C8-C7	-4.48	120.92	127.31
24	N	312	CHL	CHD-C4C-C3C	-4.48	118.26	124.84
24	N	311	CHL	C2A-C1A-CHA	-4.47	116.03	123.86
32	a	609	SQD	O7-S-C6	4.47	112.25	106.94
24	4	309	CHL	CHB-C1B-NB	-4.47	119.53	124.26
24	4	305	CHL	C2A-C1A-CHA	-4.46	116.06	123.86
31	c	615	8CT	C04-C03-C02	-4.46	116.33	122.61
24	2	310	CHL	C1D-ND-C4D	4.46	109.50	106.33
24	y	309	CHL	CHD-C4C-C3C	-4.45	118.30	124.84
24	s	414	CHL	C2A-C1A-CHA	-4.45	116.08	123.85
31	d	410	8CT	C19-C20-C21	-4.45	120.96	127.31
29	q	301	0UR	C10-C11-C12	-4.45	120.96	127.31
24	p	306	CHL	CHC-C1C-NC	4.45	130.95	124.20
24	G	318	CHL	CHB-C1B-NB	-4.45	119.55	124.26
24	q	307	CHL	CHD-C4C-C3C	-4.44	118.31	124.84
31	b	617	8CT	C01-C02-C03	-4.44	119.54	124.53
24	S	601	CHL	C2A-C1A-CHA	-4.44	116.09	123.86
24	3	305	CHL	C1D-ND-C4D	4.44	109.49	106.33
24	N	308	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
24	N	311	CHL	O2D-CGD-CBD	4.44	119.15	111.27
31	B	617	8CT	C01-C02-C03	-4.44	119.55	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	608	CHL	C1D-ND-C4D	4.43	109.48	106.33
24	G	312	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
24	Y	308	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
31	C	615	8CT	C18-C17-C16	-4.42	121.00	127.31
24	3	311	CHL	C1D-ND-C4D	4.41	109.47	106.33
27	R	615	XAT	C6-C7-C8	-4.41	116.67	125.99
31	C	613	8CT	C07-C02-C03	-4.41	116.33	122.73
24	r	307	CHL	C2A-C1A-CHA	-4.41	116.15	123.86
24	p	312	CHL	O2D-CGD-CBD	4.40	119.09	111.27
24	p	310	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
24	7	306	CHL	CHC-C1C-NC	4.40	130.88	124.20
24	9	304	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
24	6	309	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
24	7	310	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
24	3	305	CHL	C2A-C1A-CHA	-4.40	116.17	123.86
24	r	308	CHL	O2D-CGD-CBD	4.39	119.07	111.27
30	y	319	LHG	O7-C7-C8	4.38	120.95	111.50
24	N	312	CHL	C1D-ND-C4D	4.38	109.45	106.33
24	R	607	CHL	O2D-CGD-CBD	4.38	119.05	111.27
24	9	309	CHL	CHD-C4C-C3C	-4.37	118.42	124.84
31	V	401	8CT	C07-C02-C03	-4.37	116.39	122.73
31	c	613	8CT	C07-C02-C03	-4.37	116.39	122.73
24	r	307	CHL	C1D-ND-C4D	4.36	109.43	106.33
24	S	607	CHL	C2A-C1A-CHA	-4.36	116.24	123.86
24	S	605	CHL	C2A-C1A-CHA	-4.36	116.24	123.86
24	3	317	CHL	CHD-C4C-C3C	-4.36	118.43	124.84
31	S	614	8CT	C27-C26-C28	4.36	124.94	118.08
31	s	415	8CT	C27-C26-C28	4.36	124.94	118.08
24	n	312	CHL	C1D-ND-C4D	4.35	109.43	106.33
27	r	316	XAT	O4-C5-C18	4.35	120.27	115.06
31	C	614	8CT	C19-C20-C21	-4.35	121.10	127.31
31	v	401	8CT	C07-C02-C03	-4.35	116.42	122.73
24	q	309	CHL	CHB-C1B-NB	-4.35	119.66	124.26
27	R	615	XAT	O4-C5-C18	4.35	120.26	115.06
30	5	319	LHG	O7-C7-C8	4.34	120.86	111.50
24	S	601	CHL	C1D-ND-C4D	4.34	109.42	106.33
24	s	402	CHL	C2A-C1A-CHA	-4.33	116.28	123.86
24	q	309	CHL	C1D-ND-C4D	4.33	109.41	106.33
24	R	606	CHL	CHB-C1B-NB	-4.33	119.67	124.26
31	D	410	8CT	C18-C17-C16	-4.33	121.13	127.31
37	C	620	DGD	O2G-C1B-C2B	4.32	120.82	111.50
24	6	317	CHL	CHD-C4C-C3C	-4.32	118.48	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	406	CHL	C2A-C1A-CHA	-4.32	116.30	123.86
31	C	614	8CT	C04-C03-C02	-4.32	116.53	122.61
29	3	301	0UR	C10-C11-C12	-4.32	121.15	127.31
24	g	312	CHL	O2D-CGD-CBD	4.32	118.94	111.27
24	R	607	CHL	CMD-C2D-C3D	-4.32	117.69	127.61
24	G	311	CHL	CHD-C4C-C3C	-4.32	118.50	124.84
27	r	316	XAT	C6-C7-C8	-4.31	116.87	125.99
24	s	408	CHL	C1D-ND-C4D	4.31	109.40	106.33
24	3	309	CHL	CHD-C4C-C3C	-4.31	118.50	124.84
31	s	416	8CT	C28-C26-C25	4.31	125.55	118.94
31	c	614	8CT	C04-C03-C02	-4.31	116.55	122.61
24	r	308	CHL	CHA-C4D-ND	4.30	141.50	132.50
24	G	312	CHL	O2D-CGD-CBD	4.30	118.91	111.27
24	n	305	CHL	C1D-ND-C4D	4.30	109.39	106.33
30	2	319	LHG	O7-C7-C8	4.30	120.77	111.50
24	6	305	CHL	C1D-ND-C4D	4.30	109.39	106.33
24	R	607	CHL	CHA-C4D-ND	4.29	141.48	132.50
24	g	312	CHL	C2A-C1A-CHA	-4.29	116.36	123.86
24	5	310	CHL	C1D-ND-C4D	4.29	109.38	106.33
31	c	614	8CT	C19-C20-C21	-4.29	121.19	127.31
24	N	305	CHL	C1D-ND-C4D	4.29	109.38	106.33
26	u	303	0IE	C9-C10-C11	4.28	132.25	123.47
24	u	313	CHL	CMD-C2D-C3D	-4.28	117.76	127.61
24	3	311	CHL	CMD-C2D-C3D	-4.28	117.76	127.61
24	6	304	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
24	7	312	CHL	O2D-CGD-CBD	4.28	118.88	111.27
24	s	408	CHL	CHA-C4D-ND	4.28	141.45	132.50
24	5	311	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
31	C	613	8CT	C01-C02-C03	-4.28	119.73	124.53
24	s	407	CHL	C2A-C1A-CHA	-4.28	116.38	123.86
31	C	615	8CT	C04-C03-C02	-4.28	116.59	122.61
27	R	615	XAT	C26-C27-C28	-4.27	116.96	125.99
24	6	311	CHL	CHB-C1B-NB	-4.27	119.73	124.26
24	5	310	CHL	C2A-C1A-CHA	-4.27	116.39	123.85
33	i	101	LMG	O7-C10-C11	4.27	120.69	111.50
24	3	311	CHL	C2A-C1A-CHA	-4.26	116.40	123.86
24	S	606	CHL	C2A-C1A-CHA	-4.26	116.41	123.86
24	4	308	CHL	C4A-NA-C1A	4.26	108.62	106.71
24	5	313	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
24	8	304	CHL	C1D-ND-C4D	4.26	109.36	106.33
31	v	401	8CT	C04-C03-C02	-4.26	116.61	122.61
31	D	410	8CT	C19-C20-C21	-4.26	121.23	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	308	CHL	CMD-C2D-C3D	-4.26	117.83	127.61
24	2	311	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
31	s	415	8CT	C35-C30-C29	-4.25	107.32	112.70
31	X	601	8CT	C10-C11-C12	-4.25	119.81	126.23
24	Y	317	CHL	C1D-ND-C4D	4.25	109.36	106.33
24	g	313	CHL	CMD-C2D-C3D	-4.25	117.84	127.61
24	8	310	CHL	C1D-ND-C4D	4.25	109.35	106.33
24	q	311	CHL	C1D-ND-C4D	4.25	109.35	106.33
24	6	311	CHL	C1D-ND-C4D	4.25	109.35	106.33
33	d	401	LMG	O7-C10-C11	4.24	120.65	111.50
24	1	308	CHL	C4A-NA-C1A	4.24	108.61	106.71
29	3	301	0UR	C9-C8-C7	-4.24	121.26	127.31
24	S	601	CHL	CHA-C4D-ND	4.23	141.35	132.50
24	2	313	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
24	6	311	CHL	CMD-C2D-C3D	-4.23	117.88	127.61
29	N	301	0UR	C9-C8-C7	-4.23	121.28	127.31
24	3	311	CHL	CHA-C4D-ND	4.23	141.34	132.50
24	8	308	CHL	C1D-ND-C4D	4.23	109.34	106.33
31	V	401	8CT	C04-C03-C02	-4.23	116.66	122.61
24	y	309	CHL	CHA-C4D-ND	4.22	141.34	132.50
24	n	310	CHL	CHD-C4C-C3C	-4.22	118.63	124.84
24	9	317	CHL	CMD-C2D-C3D	-4.22	117.90	127.61
24	8	307	CHL	CHA-C4D-ND	4.22	141.33	132.50
24	N	317	CHL	CMD-C2D-C3D	-4.22	117.91	127.61
30	D	408	LHG	O7-C7-C8	4.22	120.59	111.50
24	p	313	CHL	CHB-C1B-NB	-4.22	119.79	124.26
24	n	308	CHL	C4A-NA-C1A	4.22	108.60	106.71
24	n	317	CHL	CMD-C2D-C3D	-4.22	117.91	127.61
24	u	305	CHL	CMD-C2D-C3D	-4.22	117.92	127.61
24	G	313	CHL	CMD-C2D-C3D	-4.21	117.92	127.61
24	s	402	CHL	CHB-C1B-NB	-4.21	119.80	124.26
24	u	318	CHL	CMD-C2D-C3D	-4.21	117.93	127.61
24	u	312	CHL	CHA-C4D-ND	4.21	141.30	132.50
29	n	301	0UR	C9-C8-C7	-4.21	121.30	127.31
27	r	316	XAT	C26-C27-C28	-4.21	117.10	125.99
24	Y	310	CHL	C1D-ND-C4D	4.21	109.32	106.33
24	s	402	CHL	CHA-C4D-ND	4.21	141.30	132.50
24	q	307	CHL	CHA-C4D-ND	4.21	141.30	132.50
24	7	313	CHL	CHB-C1B-NB	-4.21	119.81	124.26
24	s	402	CHL	CHC-C1C-NC	4.21	130.58	124.20
24	R	606	CHL	C1D-ND-C4D	4.20	109.32	106.33
24	p	312	CHL	CHA-C4D-ND	4.20	141.29	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	311	CHL	CHA-C4D-ND	4.20	141.29	132.50
24	1	309	CHL	CMD-C2D-C3D	-4.20	117.95	127.61
24	Y	310	CHL	CHA-C4D-ND	4.20	141.28	132.50
24	Y	308	CHL	CHA-C4D-ND	4.20	141.28	132.50
24	q	308	CHL	CHA-C4D-ND	4.20	141.28	132.50
24	s	409	CHL	C1D-ND-C4D	4.20	109.32	106.33
24	N	310	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
24	S	601	CHL	CHC-C1C-NC	4.20	130.57	124.20
24	9	311	CHL	CHA-C4D-ND	4.19	141.28	132.50
31	S	614	8CT	C35-C30-C29	-4.19	107.40	112.70
24	4	309	CHL	CMD-C2D-C3D	-4.19	117.97	127.61
24	y	310	CHL	CHA-C4D-ND	4.19	141.26	132.50
24	4	305	CHL	CHB-C1B-NB	-4.19	119.82	124.26
24	7	312	CHL	CHC-C1C-NC	4.19	130.56	124.20
24	R	608	CHL	CHB-C1B-NB	-4.19	119.82	124.26
24	8	308	CHL	CHA-C4D-ND	4.19	141.25	132.50
24	9	312	CHL	CMD-C2D-C3D	-4.19	117.99	127.61
24	R	601	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
24	7	312	CHL	CHA-C4D-ND	4.18	141.25	132.50
24	s	414	CHL	CHB-C1B-NB	-4.18	119.83	124.26
33	m	101	LMG	O7-C10-C11	4.18	120.51	111.50
24	N	312	CHL	CHB-C1B-NB	-4.18	119.83	124.26
24	9	305	CHL	C1D-ND-C4D	4.18	109.30	106.33
31	S	615	8CT	C28-C26-C25	4.18	125.35	118.94
24	u	311	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
24	n	317	CHL	CHA-C4D-ND	4.18	141.24	132.50
24	1	312	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
24	N	311	CHL	CHA-C4D-ND	4.17	141.23	132.50
24	Y	319	CHL	C1D-ND-C4D	4.17	109.30	106.33
24	q	308	CHL	CMD-C2D-C3D	-4.17	118.02	127.61
24	2	312	CHL	CHA-C4D-ND	4.17	141.22	132.50
24	8	308	CHL	CMD-C2D-C3D	-4.17	118.03	127.61
24	n	308	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
24	6	308	CHL	C4A-NA-C1A	4.17	108.58	106.71
24	2	310	CHL	CHB-C1B-NB	-4.16	119.85	124.26
24	r	302	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
24	G	318	CHL	C2A-C1A-CHA	-4.16	116.59	123.85
24	N	311	CHL	C1D-ND-C4D	4.16	109.29	106.33
24	u	306	CHL	C1D-ND-C4D	4.16	109.29	106.33
24	2	318	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
24	5	313	CHL	C2A-C1A-CHA	-4.16	116.59	123.85
24	G	312	CHL	C2A-C1A-CHA	-4.16	116.59	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	308	CHL	CHA-C4D-ND	4.15	141.19	132.50
24	s	408	CHL	OBD-CAD-C3D	-4.15	118.53	128.52
24	9	304	CHL	CMD-C2D-C3D	-4.15	118.06	127.61
24	q	308	CHL	C1D-ND-C4D	4.15	109.28	106.33
24	N	317	CHL	CHA-C4D-ND	4.15	141.18	132.50
24	4	312	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
24	1	305	CHL	CHB-C1B-NB	-4.15	119.87	124.26
24	4	308	CHL	CHA-C4D-ND	4.15	141.17	132.50
24	5	312	CHL	CHA-C4D-ND	4.15	141.17	132.50
24	4	317	CHL	CHA-C4D-ND	4.14	141.17	132.50
24	s	408	CHL	C2A-C1A-CHA	-4.14	116.61	123.86
24	y	311	CHL	C1D-ND-C4D	4.14	109.28	106.33
24	S	613	CHL	CHB-C1B-NB	-4.14	119.87	124.26
24	n	311	CHL	CHA-C4D-ND	4.14	141.16	132.50
29	N	301	0UR	C5-C4-C3	-4.14	122.03	127.00
24	Y	309	CHL	CHA-C4D-ND	4.14	141.16	132.50
24	Y	304	CHL	CHA-C4D-ND	4.14	141.15	132.50
24	g	311	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
24	u	310	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
24	3	308	CHL	CHA-C4D-ND	4.13	141.15	132.50
24	y	311	CHL	CHA-C4D-ND	4.13	141.15	132.50
24	g	310	CHL	CHD-C4C-C3C	-4.13	118.76	124.84
24	2	309	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
24	5	309	CHL	CHA-C4D-ND	4.13	141.14	132.50
31	s	415	8CT	C07-C02-C03	-4.13	116.73	122.73
24	g	305	CHL	CHA-C4D-ND	4.13	141.14	132.50
24	2	309	CHL	CHA-C4D-ND	4.13	141.14	132.50
24	s	408	CHL	CHB-C1B-NB	-4.13	119.89	124.26
24	u	305	CHL	CHA-C4D-ND	4.13	141.14	132.50
24	u	318	CHL	CHA-C4D-ND	4.13	141.14	132.50
24	3	312	CHL	CMD-C2D-C3D	-4.13	118.11	127.61
24	9	310	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
24	S	607	CHL	CHA-C4D-ND	4.13	141.13	132.50
24	Y	317	CHL	CHA-C4D-ND	4.13	141.13	132.50
24	y	305	CHL	CHA-C4D-ND	4.13	141.13	132.50
24	2	310	CHL	C2A-C1A-CHA	-4.13	116.65	123.85
31	s	416	8CT	C27-C26-C25	-4.12	117.14	122.92
24	G	305	CHL	CHA-C4D-ND	4.12	141.13	132.50
24	3	317	CHL	CHA-C4D-ND	4.12	141.13	132.50
24	G	310	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
33	C	618	LMG	O7-C10-C11	4.12	120.39	111.50
24	y	318	CHL	C1D-ND-C4D	4.12	109.26	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	311	CHL	C1D-ND-C4D	4.12	109.26	106.33
24	2	312	CHL	C1D-ND-C4D	4.12	109.26	106.33
24	4	309	CHL	CHD-C4C-C3C	-4.12	118.79	124.84
24	2	318	CHL	CHA-C4D-ND	4.12	141.11	132.50
24	p	305	CHL	CMD-C2D-C3D	-4.12	118.14	127.61
24	2	310	CHL	CHA-C4D-ND	4.12	141.11	132.50
24	3	317	CHL	CMD-C2D-C3D	-4.12	118.15	127.61
24	N	304	CHL	CHD-C4C-C3C	-4.11	118.79	124.84
24	S	605	CHL	CHA-C4D-ND	4.11	141.11	132.50
31	x	601	8CT	C10-C11-C12	-4.11	120.02	126.23
24	g	318	CHL	CHA-C4D-ND	4.11	141.10	132.50
24	n	312	CHL	CHB-C1B-NB	-4.11	119.90	124.26
24	5	318	CHL	CHA-C4D-ND	4.11	141.10	132.50
33	D	401	LMG	O7-C10-C11	4.11	120.36	111.50
24	u	310	CHL	CMD-C2D-C3D	-4.11	118.16	127.61
24	1	317	CHL	CHA-C4D-ND	4.11	141.10	132.50
24	4	310	CHL	C2A-C1A-CHA	-4.11	116.67	123.86
24	Y	319	CHL	CHB-C1B-NB	-4.11	119.91	124.26
24	N	309	CHL	CHA-C4D-ND	4.11	141.10	132.50
26	p	303	0IE	C23-C16-C15	-4.11	117.17	122.92
24	8	315	CHL	CHA-C4D-ND	4.11	141.09	132.50
24	2	305	CHL	CHA-C4D-ND	4.11	141.09	132.50
31	S	615	8CT	C14-C13-C12	-4.11	121.45	127.31
24	6	309	CHL	C2A-C1A-CHA	-4.11	116.68	123.86
24	1	308	CHL	CHA-C4D-ND	4.11	141.09	132.50
24	q	316	CHL	CHA-C4D-ND	4.11	141.09	132.50
24	y	312	CHL	O2D-CGD-CBD	4.11	118.56	111.27
24	g	309	CHL	CHA-C4D-ND	4.11	141.09	132.50
24	4	311	CHL	CMD-C2D-C3D	-4.10	118.17	127.61
24	Y	311	CHL	O2D-CGD-CBD	4.10	118.56	111.27
24	6	312	CHL	CMD-C2D-C3D	-4.10	118.17	127.61
24	g	310	CHL	CMD-C2D-C3D	-4.10	118.17	127.61
24	6	317	CHL	CMD-C2D-C3D	-4.10	118.18	127.61
24	5	310	CHL	CHA-C4D-ND	4.10	141.08	132.50
24	r	309	CHL	CHB-C1B-NB	-4.10	119.91	124.26
24	s	406	CHL	CHA-C4D-ND	4.10	141.08	132.50
24	p	309	CHL	CHA-C4D-ND	4.10	141.08	132.50
24	9	317	CHL	CHA-C4D-ND	4.10	141.08	132.50
29	Y	301	0UR	C34-C27-C1	-4.10	119.11	124.49
31	d	410	8CT	C01-C02-C03	-4.10	119.92	124.53
24	g	309	CHL	CMD-C2D-C3D	-4.10	118.19	127.61
26	Y	303	0IE	C23-C16-C15	-4.10	117.18	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	312	CHL	CHC-C1C-NC	4.10	130.42	124.20
24	G	310	CHL	CMD-C2D-C3D	-4.10	118.19	127.61
26	y	303	0IE	C23-C16-C15	-4.10	117.19	122.92
24	q	303	CHL	CHA-C4D-ND	4.10	141.07	132.50
26	u	303	0IE	C23-C16-C15	-4.09	117.19	122.92
26	7	303	0IE	C23-C16-C15	-4.09	117.19	122.92
24	5	318	CHL	CHD-C4C-C3C	-4.09	118.82	124.84
24	G	318	CHL	CHA-C4D-ND	4.09	141.06	132.50
24	1	310	CHL	C2A-C1A-CHA	-4.09	116.70	123.86
24	1	304	CHL	CHA-C4D-ND	4.09	141.06	132.50
24	8	303	CHL	CHA-C4D-ND	4.09	141.06	132.50
24	6	317	CHL	CHA-C4D-ND	4.09	141.06	132.50
24	7	311	CHL	C2A-C1A-CHA	-4.09	116.71	123.86
24	g	306	CHL	CMD-C2D-C3D	-4.09	118.20	127.61
24	9	308	CHL	CHA-C4D-ND	4.09	141.06	132.50
24	5	313	CHL	CMD-C2D-C3D	-4.09	118.21	127.61
24	u	309	CHL	CHA-C4D-ND	4.09	141.05	132.50
24	q	310	CHL	CHA-C4D-ND	4.09	141.05	132.50
24	Y	312	CHL	CHA-C4D-ND	4.09	141.05	132.50
31	c	613	8CT	C01-C02-C03	-4.08	119.94	124.53
24	Y	311	CHL	CHC-C1C-NC	4.08	130.40	124.20
24	6	304	CHL	CHA-C4D-ND	4.08	141.04	132.50
24	G	306	CHL	C1D-ND-C4D	4.08	109.24	106.33
24	7	309	CHL	CHA-C4D-ND	4.08	141.04	132.50
24	n	304	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
24	y	310	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
24	1	309	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
24	8	303	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
24	R	601	CHL	CHA-C4D-ND	4.08	141.04	132.50
27	R	615	XAT	C35-C34-C33	-4.08	121.48	127.31
24	N	304	CHL	CHA-C4D-ND	4.08	141.03	132.50
24	y	309	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
24	G	309	CHL	CHA-C4D-ND	4.08	141.03	132.50
29	q	301	0UR	C9-C8-C7	-4.08	121.49	127.31
24	8	309	CHL	CHA-C4D-ND	4.08	141.03	132.50
24	5	305	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
24	n	309	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
24	p	309	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
24	7	309	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
24	n	304	CHL	CHA-C4D-ND	4.08	141.03	132.50
24	G	306	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
24	s	414	CHL	C1D-ND-C4D	4.08	109.23	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	303	0IE	C10-C9-C8	4.08	131.82	123.47
24	q	304	CHL	C1D-ND-C4D	4.08	109.23	106.33
24	G	309	CHL	CMD-C2D-C3D	-4.07	118.24	127.61
24	y	313	CHL	CMD-C2D-C3D	-4.07	118.24	127.61
24	9	309	CHL	CMD-C2D-C3D	-4.07	118.24	127.61
24	7	305	CHL	CHA-C4D-ND	4.07	141.02	132.50
24	4	310	CHL	CHA-C4D-ND	4.07	141.02	132.50
24	p	305	CHL	CHA-C4D-ND	4.07	141.02	132.50
24	n	309	CHL	CHA-C4D-ND	4.07	141.02	132.50
24	1	311	CHL	CMD-C2D-C3D	-4.07	118.25	127.61
29	6	301	0UR	C9-C8-C7	-4.07	121.50	127.31
24	N	312	CHL	CMD-C2D-C3D	-4.07	118.25	127.61
24	8	315	CHL	CMD-C2D-C3D	-4.07	118.25	127.61
26	G	303	0IE	C10-C9-C8	4.07	131.81	123.47
24	q	303	CHL	CHD-C4C-C3C	-4.07	118.86	124.84
24	2	313	CHL	C2A-C1A-CHA	-4.07	116.75	123.85
24	5	305	CHL	CHA-C4D-ND	4.07	141.01	132.50
24	n	312	CHL	CMD-C2D-C3D	-4.07	118.26	127.61
24	q	316	CHL	CHD-C4C-C3C	-4.07	118.86	124.84
24	y	318	CHL	CHA-C4D-ND	4.07	141.01	132.50
24	r	302	CHL	CHA-C4D-ND	4.07	141.01	132.50
24	7	305	CHL	CMD-C2D-C3D	-4.07	118.26	127.61
24	7	318	CHL	CHA-C4D-ND	4.06	141.00	132.50
24	S	608	CHL	CMD-C2D-C3D	-4.06	118.27	127.61
24	y	312	CHL	CHA-C4D-ND	4.06	141.00	132.50
24	5	318	CHL	C4A-NA-C1A	4.06	108.53	106.71
30	7	319	LHG	O7-C7-C8	4.06	120.25	111.50
37	c	619	DGD	O2G-C1B-C2B	4.06	120.25	111.50
24	4	304	CHL	CHA-C4D-ND	4.06	140.99	132.50
24	4	317	CHL	CMD-C2D-C3D	-4.06	118.27	127.61
24	2	305	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
24	n	311	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
24	2	313	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
31	S	615	8CT	C27-C26-C25	-4.06	117.24	122.92
24	3	308	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
24	s	402	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
24	Y	308	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
29	n	301	0UR	C5-C4-C3	-4.06	122.13	127.00
24	6	304	CHL	CMD-C2D-C3D	-4.05	118.29	127.61
24	3	304	CHL	CHA-C4D-ND	4.05	140.98	132.50
24	Y	312	CHL	CMD-C2D-C3D	-4.05	118.29	127.61
24	5	309	CHL	CHD-C4C-C3C	-4.05	118.88	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	311	CHL	CMD-C2D-C3D	-4.05	118.29	127.61
24	p	318	CHL	CHA-C4D-ND	4.05	140.97	132.50
24	5	312	CHL	CMD-C2D-C3D	-4.05	118.30	127.61
24	g	318	CHL	C2A-C1A-CHA	-4.05	116.78	123.85
24	8	310	CHL	CHC-C1C-NC	4.05	130.35	124.20
24	1	310	CHL	CHA-C4D-ND	4.05	140.97	132.50
24	1	304	CHL	CMD-C2D-C3D	-4.05	118.30	127.61
31	S	615	8CT	C07-C02-C03	-4.05	116.86	122.73
24	y	313	CHL	CHA-C4D-ND	4.05	140.96	132.50
30	a	612	LHG	O7-C7-C8	4.05	120.22	111.50
24	s	409	CHL	CMD-C2D-C3D	-4.04	118.31	127.61
24	9	304	CHL	CHA-C4D-ND	4.04	140.96	132.50
24	S	608	CHL	CHC-C1C-NC	4.04	130.34	124.20
24	q	303	CHL	CMD-C2D-C3D	-4.04	118.31	127.61
24	R	606	CHL	CHA-C4D-ND	4.04	140.96	132.50
24	N	308	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	u	305	CHL	CHD-C4C-C3C	-4.04	118.90	124.84
24	3	309	CHL	C2A-C1A-CHA	-4.04	116.79	123.86
24	7	313	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	S	601	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	n	304	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	9	308	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	5	305	CHL	C2A-C1A-CHA	-4.04	116.79	123.86
31	a	608	8CT	C10-C11-C12	-4.04	120.13	126.23
24	S	613	CHL	CHA-C4D-ND	4.04	140.95	132.50
31	A	608	8CT	C10-C11-C12	-4.04	120.13	126.23
24	2	312	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	G	311	CHL	CMD-C2D-C3D	-4.04	118.32	127.61
24	s	414	CHL	CHA-C4D-ND	4.04	140.95	132.50
24	1	317	CHL	CMD-C2D-C3D	-4.04	118.33	127.61
29	y	301	0UR	C34-C27-C1	-4.04	119.19	124.49
24	Y	319	CHL	CHA-C4D-ND	4.04	140.94	132.50
24	G	310	CHL	C2A-C1A-CHA	-4.03	116.80	123.86
24	r	306	CHL	CHA-C4D-ND	4.03	140.94	132.50
24	9	305	CHL	CHC-C1C-NC	4.03	130.32	124.20
24	3	304	CHL	CMD-C2D-C3D	-4.03	118.34	127.61
30	A	612	LHG	O7-C7-C8	4.03	120.19	111.50
24	Y	311	CHL	CHA-C4D-ND	4.03	140.93	132.50
24	1	308	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
24	7	310	CHL	CMD-C2D-C3D	-4.03	118.34	127.61
24	3	310	CHL	CMD-C2D-C3D	-4.03	118.35	127.61
30	p	319	LHG	O7-C7-C8	4.03	120.18	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	319	LHG	O7-C7-C8	4.03	120.18	111.50
24	Y	309	CHL	CMD-C2D-C3D	-4.03	118.35	127.61
30	C	617	LHG	O7-C7-C8	4.03	120.18	111.50
26	g	303	0IE	C10-C9-C8	4.02	131.72	123.47
24	p	311	CHL	C2A-C1A-CHA	-4.02	116.82	123.86
24	Y	319	CHL	CMD-C2D-C3D	-4.02	118.36	127.61
28	r	317	NEX	C11-C10-C9	-4.02	121.57	127.31
24	p	313	CHL	CMD-C2D-C3D	-4.02	118.36	127.61
24	N	310	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
24	7	305	CHL	C3B-C4B-NB	4.02	114.24	110.52
24	8	303	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
28	R	616	NEX	C11-C10-C9	-4.02	121.58	127.31
24	S	606	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
24	6	308	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
24	9	311	CHL	CMD-C2D-C3D	-4.02	118.38	127.61
24	u	309	CHL	CMD-C2D-C3D	-4.02	118.38	127.61
24	8	304	CHL	CHA-C4D-ND	4.02	140.90	132.50
24	N	304	CHL	CMD-C2D-C3D	-4.01	118.38	127.61
24	N	309	CHL	CMD-C2D-C3D	-4.01	118.38	127.61
24	3	308	CHL	C4A-NA-C1A	4.01	108.51	106.71
24	6	310	CHL	CMD-C2D-C3D	-4.01	118.38	127.61
24	u	313	CHL	CHA-C4D-ND	4.01	140.89	132.50
31	x	601	8CT	C25-C24-C23	-4.01	110.69	123.22
24	S	605	CHL	CMD-C2D-C3D	-4.01	118.39	127.61
33	B	619	LMG	C8-O7-C10	-4.01	107.92	117.79
24	u	312	CHL	CMD-C2D-C3D	-4.01	118.39	127.61
31	C	613	8CT	C04-C03-C02	-4.01	116.97	122.61
24	R	605	CHL	CHA-C4D-ND	4.01	140.89	132.50
31	X	601	8CT	C25-C24-C23	-4.01	110.71	123.22
24	7	310	CHL	CHA-C4D-ND	4.01	140.88	132.50
31	S	614	8CT	C07-C02-C03	-4.01	116.92	122.73
24	q	316	CHL	CMD-C2D-C3D	-4.00	118.41	127.61
24	S	606	CHL	CHA-C4D-ND	4.00	140.87	132.50
24	q	309	CHL	CHA-C4D-ND	4.00	140.87	132.50
30	c	617	LHG	O7-C7-C8	4.00	120.13	111.50
24	s	406	CHL	CMD-C2D-C3D	-4.00	118.41	127.61
24	5	310	CHL	CHB-C1B-NB	-4.00	120.02	124.26
24	9	312	CHL	CHA-C4D-ND	4.00	140.87	132.50
24	g	311	CHL	CMD-C2D-C3D	-4.00	118.41	127.61
27	r	316	XAT	C35-C34-C33	-4.00	121.60	127.31
24	r	307	CHL	CHA-C4D-ND	4.00	140.87	132.50
30	g	319	LHG	O7-C7-C8	4.00	120.12	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	311	CHL	C1D-ND-C4D	4.00	109.18	106.33
24	9	310	CHL	CHA-C4D-ND	4.00	140.86	132.50
24	q	304	CHL	CHA-C4D-ND	4.00	140.86	132.50
24	4	305	CHL	CHA-C4D-ND	4.00	140.86	132.50
24	4	308	CHL	CHD-C4C-C3C	-4.00	118.97	124.84
24	g	312	CHL	CHA-C4D-ND	4.00	140.86	132.50
24	p	310	CHL	CHA-C4D-ND	4.00	140.86	132.50
24	s	407	CHL	CHA-C4D-ND	3.99	140.85	132.50
24	n	308	CHL	CHA-C4D-ND	3.99	140.85	132.50
32	D	409	SQD	O9-S-C6	3.99	111.68	106.94
31	D	410	8CT	C24-C25-C26	-3.99	121.61	127.31
24	s	407	CHL	CMD-C2D-C3D	-3.99	118.43	127.61
26	y	303	0IE	C10-C9-C8	3.99	131.65	123.47
24	S	613	CHL	C1D-ND-C4D	3.99	109.17	106.33
26	3	303	0IE	C23-C16-C15	-3.99	117.33	122.92
24	N	311	CHL	CHB-C1B-NB	-3.99	120.03	124.26
24	5	312	CHL	C1D-ND-C4D	3.99	109.17	106.33
24	q	311	CHL	CHC-C1C-NC	3.99	130.25	124.20
28	1	303	NEX	C11-C10-C9	-3.99	121.62	127.31
28	G	304	NEX	C11-C10-C9	-3.99	121.62	127.31
29	G	301	0UR	C9-C8-C7	-3.99	121.62	127.31
32	d	409	SQD	O9-S-C6	3.99	111.68	106.94
37	C	619	DGD	O2G-C1B-C2B	3.99	120.09	111.50
24	u	311	CHL	CHA-C4D-ND	3.99	140.84	132.50
24	S	607	CHL	C1D-ND-C4D	3.99	109.17	106.33
24	4	308	CHL	CMD-C2D-C3D	-3.98	118.45	127.61
31	s	415	8CT	C28-C26-C25	-3.98	112.83	118.94
24	S	608	CHL	C1D-ND-C4D	3.98	109.16	106.33
24	1	309	CHL	CHA-C4D-ND	3.98	140.83	132.50
26	p	302	0IE	C4-C3-C2	-3.98	116.66	120.08
31	S	614	8CT	C28-C26-C25	-3.98	112.83	118.94
24	1	308	CHL	CMD-C2D-C3D	-3.98	118.46	127.61
24	5	309	CHL	CMD-C2D-C3D	-3.98	118.46	127.61
28	y	304	NEX	C11-C10-C9	-3.98	121.63	127.31
32	d	409	SQD	O7-S-C6	3.98	111.67	106.94
24	g	306	CHL	CHA-C4D-ND	3.98	140.82	132.50
31	d	410	8CT	C24-C25-C26	-3.98	121.63	127.31
24	9	305	CHL	CHB-C1B-NB	-3.98	120.05	124.26
24	1	311	CHL	CHA-C4D-ND	3.98	140.82	132.50
24	1	312	CHL	C2A-C1A-CHA	-3.98	116.91	123.86
24	9	310	CHL	CMD-C2D-C3D	-3.98	118.47	127.61
24	u	311	CHL	CMD-C2D-C3D	-3.98	118.47	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	305	CHL	C3B-C4B-NB	3.98	114.20	110.52
24	2	311	CHL	CMD-C2D-C3D	-3.97	118.47	127.61
24	4	311	CHL	CHA-C4D-ND	3.97	140.81	132.50
24	g	310	CHL	CHA-C4D-ND	3.97	140.81	132.50
24	G	312	CHL	CHA-C4D-ND	3.97	140.81	132.50
31	A	608	8CT	C19-C20-C21	-3.97	121.64	127.31
24	n	310	CHL	CMD-C2D-C3D	-3.97	118.47	127.61
24	u	310	CHL	CHA-C4D-ND	3.97	140.81	132.50
24	N	308	CHL	CHA-C4D-ND	3.97	140.81	132.50
24	1	305	CHL	CHA-C4D-ND	3.97	140.81	132.50
31	s	416	8CT	C14-C13-C12	-3.97	121.64	127.31
24	4	309	CHL	CHA-C4D-ND	3.97	140.81	132.50
24	N	310	CHL	CHA-C4D-ND	3.97	140.81	132.50
24	p	310	CHL	CMD-C2D-C3D	-3.97	118.48	127.61
24	p	312	CHL	CHC-C1C-NC	3.97	130.23	124.20
24	G	305	CHL	CMD-C2D-C3D	-3.97	118.48	127.61
30	9	318	LHG	O7-C7-C8	3.97	120.06	111.50
24	5	313	CHL	CHA-C4D-ND	3.97	140.80	132.50
24	2	313	CHL	CHA-C4D-ND	3.97	140.80	132.50
24	6	310	CHL	CHA-C4D-ND	3.97	140.80	132.50
31	D	410	8CT	C01-C02-C03	-3.97	120.07	124.53
28	g	304	NEX	C11-C10-C9	-3.97	121.65	127.31
24	S	601	CHL	CHB-C1B-NB	-3.97	120.06	124.26
24	R	605	CHL	CMD-C2D-C3D	-3.97	118.49	127.61
24	7	311	CHL	CHA-C4D-ND	3.97	140.79	132.50
24	r	306	CHL	CMD-C2D-C3D	-3.96	118.49	127.61
24	3	308	CHL	CHD-C4C-C3C	-3.96	119.01	124.84
24	2	306	CHL	C1D-ND-C4D	3.96	109.15	106.33
29	8	301	0UR	C9-C8-C7	-3.96	121.65	127.31
24	G	306	CHL	CHA-C4D-ND	3.96	140.79	132.50
31	x	601	8CT	C18-C19-C20	-3.96	115.36	123.47
24	2	309	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
24	G	310	CHL	CHA-C4D-ND	3.96	140.79	132.50
24	n	310	CHL	CHA-C4D-ND	3.96	140.79	132.50
24	8	315	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
24	6	309	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
24	9	309	CHL	CHA-C4D-ND	3.96	140.78	132.50
24	n	309	CHL	C3B-C4B-NB	3.96	114.19	110.52
28	N	303	NEX	C11-C10-C9	-3.96	121.66	127.31
24	3	304	CHL	C2A-C1A-CHA	-3.96	116.94	123.86
26	G	302	0IE	C23-C16-C15	-3.96	117.38	122.92
24	n	309	CHL	CHC-C1C-NC	3.96	130.21	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	309	CHL	CMD-C2D-C3D	-3.96	118.51	127.61
31	a	608	8CT	C19-C20-C21	-3.96	121.66	127.31
24	g	313	CHL	CHA-C4D-ND	3.95	140.77	132.50
28	n	303	NEX	C11-C10-C9	-3.95	121.67	127.31
24	N	309	CHL	CHC-C1C-NC	3.95	130.20	124.20
28	4	303	NEX	C11-C10-C9	-3.95	121.67	127.31
28	7	304	NEX	C11-C10-C9	-3.95	121.67	127.31
24	3	310	CHL	CHA-C4D-ND	3.95	140.76	132.50
24	p	311	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
26	g	302	0IE	C23-C16-C15	-3.95	117.39	122.92
24	2	318	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
24	5	318	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
24	n	308	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
28	p	304	NEX	C11-C10-C9	-3.95	121.68	127.31
31	c	613	8CT	C10-C11-C12	-3.95	120.27	126.23
28	5	304	NEX	C11-C10-C9	-3.95	121.68	127.31
24	8	310	CHL	CMD-C2D-C3D	-3.95	118.54	127.61
24	4	312	CHL	CMD-C2D-C3D	-3.95	118.54	127.61
24	7	305	CHL	CHC-C1C-NC	3.95	130.19	124.20
28	3	318	NEX	C11-C10-C9	-3.94	121.68	127.31
24	4	305	CHL	C1D-ND-C4D	3.94	109.14	106.33
24	n	312	CHL	CHA-C4D-ND	3.94	140.74	132.50
24	G	311	CHL	CHA-C4D-ND	3.94	140.74	132.50
24	r	309	CHL	CHA-C4D-ND	3.94	140.74	132.50
24	5	306	CHL	C1D-ND-C4D	3.94	109.13	106.33
29	g	301	0UR	C9-C8-C7	-3.94	121.69	127.31
29	u	301	0UR	C14-C15-C16	-3.94	121.69	127.31
28	6	303	NEX	C11-C10-C9	-3.94	121.69	127.31
24	8	309	CHL	CMD-C2D-C3D	-3.94	118.56	127.61
24	q	311	CHL	CMD-C2D-C3D	-3.94	118.56	127.61
24	4	304	CHL	CMD-C2D-C3D	-3.94	118.56	127.61
24	6	305	CHL	CMD-C2D-C3D	-3.93	118.56	127.61
24	7	306	CHL	CHA-C4D-ND	3.93	140.73	132.50
29	Y	301	0UR	C10-C11-C12	-3.93	121.69	127.31
24	6	309	CHL	CHC-C1C-NC	3.93	130.17	124.20
24	G	313	CHL	CHA-C4D-ND	3.93	140.73	132.50
30	1	318	LHG	O7-C7-C8	3.93	119.98	111.50
24	4	304	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
24	p	306	CHL	CHA-C4D-ND	3.93	140.72	132.50
24	4	305	CHL	CMD-C2D-C3D	-3.93	118.57	127.61
24	u	306	CHL	CHB-C1B-NB	-3.93	120.10	124.26
24	g	305	CHL	CMD-C2D-C3D	-3.93	118.57	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	310	CHL	CMD-C2D-C3D	-3.93	118.57	127.61
37	c	618	DGD	O2G-C1B-C2B	3.93	119.97	111.50
24	r	306	CHL	C2A-C1A-CHA	-3.93	116.99	123.85
28	r	301	NEX	C11-C10-C9	-3.93	121.70	127.31
29	7	301	0UR	C10-C11-C12	-3.93	121.70	127.31
24	s	409	CHL	CHA-C4D-ND	3.93	140.72	132.50
32	b	618	SQD	O47-C7-C8	3.93	119.97	111.50
31	C	615	8CT	C07-C02-C03	-3.93	117.03	122.73
24	q	311	CHL	CHA-C4D-ND	3.93	140.72	132.50
24	q	304	CHL	CMD-C2D-C3D	-3.93	118.58	127.61
28	s	401	NEX	C11-C10-C9	-3.93	121.71	127.31
33	D	411	LMG	O7-C10-C11	3.93	119.96	111.50
24	1	311	CHL	C1D-ND-C4D	3.92	109.12	106.33
30	4	318	LHG	O7-C7-C8	3.92	119.96	111.50
24	1	312	CHL	CHA-C4D-ND	3.92	140.71	132.50
24	R	608	CHL	CHA-C4D-ND	3.92	140.71	132.50
24	6	309	CHL	CHA-C4D-ND	3.92	140.71	132.50
24	q	307	CHL	CMD-C2D-C3D	-3.92	118.59	127.61
24	6	308	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
26	9	302	0IE	C23-C16-C15	-3.92	117.43	122.92
24	7	313	CHL	CHA-C4D-ND	3.92	140.70	132.50
24	5	311	CHL	CMD-C2D-C3D	-3.92	118.59	127.61
24	s	409	CHL	CHC-C1C-NC	3.92	130.15	124.20
26	9	303	0IE	C23-C16-C15	-3.92	117.43	122.92
24	R	601	CHL	CMD-C2D-C3D	-3.92	118.59	127.61
24	8	310	CHL	CHA-C4D-ND	3.92	140.70	132.50
24	g	310	CHL	C2A-C1A-CHA	-3.92	117.00	123.86
31	s	416	8CT	C07-C02-C03	-3.92	117.04	122.73
26	7	302	0IE	C4-C3-C2	-3.92	116.72	120.08
28	S	617	NEX	C11-C10-C9	-3.92	121.72	127.31
24	r	302	CHL	CMD-C2D-C3D	-3.92	118.60	127.61
24	7	311	CHL	CMD-C2D-C3D	-3.92	118.60	127.61
24	S	602	CHL	CHA-C4D-ND	3.92	140.69	132.50
24	4	311	CHL	CHB-C1B-NB	-3.92	120.11	124.26
29	y	301	0UR	C10-C11-C12	-3.92	121.72	127.31
24	6	305	CHL	CHA-C4D-ND	3.92	140.69	132.50
32	D	409	SQD	O7-S-C6	3.92	111.59	106.94
24	8	304	CHL	CMD-C2D-C3D	-3.91	118.61	127.61
24	4	312	CHL	CHA-C4D-ND	3.91	140.69	132.50
26	5	302	0IE	C23-C16-C15	-3.91	117.44	122.92
24	N	312	CHL	CHA-C4D-ND	3.91	140.69	132.50
24	y	306	CHL	CAC-C3C-C4C	3.91	129.89	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	305	CHL	CMD-C2D-C3D	-3.91	118.61	127.61
32	B	618	SQD	O47-C7-C8	3.91	119.93	111.50
28	9	319	NEX	C11-C10-C9	-3.91	121.73	127.31
24	R	607	CHL	C1D-ND-C4D	3.91	109.11	106.33
24	p	305	CHL	CHC-C1C-NC	3.91	130.13	124.20
26	5	303	0IE	C9-C10-C11	3.91	131.48	123.47
24	1	305	CHL	C1D-ND-C4D	3.91	109.11	106.33
24	N	305	CHL	CHA-C4D-ND	3.91	140.68	132.50
24	1	312	CHL	CMD-C2D-C3D	-3.91	118.62	127.61
24	3	310	CHL	CHD-C4C-C3C	-3.91	119.10	124.84
24	y	311	CHL	CHC-C1C-NC	3.91	130.13	124.20
24	g	311	CHL	CHA-C4D-ND	3.91	140.67	132.50
24	G	318	CHL	CMD-C2D-C3D	-3.91	118.63	127.61
24	2	305	CHL	C2A-C1A-CHA	-3.91	117.03	123.86
24	Y	305	CHL	CHA-C4D-ND	3.91	140.67	132.50
24	4	312	CHL	C2A-C1A-CHA	-3.90	117.03	123.86
24	g	318	CHL	CMD-C2D-C3D	-3.90	118.63	127.61
24	n	305	CHL	CHA-C4D-ND	3.90	140.67	132.50
28	2	304	NEX	C11-C10-C9	-3.90	121.74	127.31
31	c	615	8CT	C07-C02-C03	-3.90	117.06	122.73
26	g	303	0IE	C23-C16-C15	-3.90	117.46	122.92
24	5	306	CHL	CHA-C4D-ND	3.90	140.66	132.50
24	p	311	CHL	CHA-C4D-ND	3.90	140.66	132.50
24	2	311	CHL	CHA-C4D-ND	3.90	140.66	132.50
26	u	302	0IE	C23-C16-C15	-3.90	117.46	122.92
24	R	602	CHL	CMD-C2D-C3D	-3.90	118.64	127.61
24	3	309	CHL	CHA-C4D-ND	3.90	140.66	132.50
24	S	608	CHL	CHA-C4D-ND	3.90	140.66	132.50
24	6	312	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
24	3	305	CHL	CHA-C4D-ND	3.90	140.66	132.50
24	p	313	CHL	CHA-C4D-ND	3.90	140.66	132.50
31	X	601	8CT	C18-C19-C20	-3.90	115.49	123.47
24	8	307	CHL	CMD-C2D-C3D	-3.90	118.65	127.61
24	2	306	CHL	CHA-C4D-ND	3.90	140.65	132.50
24	6	312	CHL	CHA-C4D-ND	3.90	140.65	132.50
24	G	312	CHL	CMD-C2D-C3D	-3.90	118.65	127.61
24	Y	304	CHL	CMD-C2D-C3D	-3.90	118.65	127.61
26	G	303	0IE	C23-C16-C15	-3.90	117.47	122.92
24	g	312	CHL	CMD-C2D-C3D	-3.90	118.65	127.61
28	u	304	NEX	C11-C10-C9	-3.90	121.75	127.31
24	S	607	CHL	CMD-C2D-C3D	-3.89	118.66	127.61
24	y	306	CHL	CHA-C4D-ND	3.89	140.64	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	312	CHL	CHA-C4D-ND	3.89	140.64	132.50
24	Y	305	CHL	CAC-C3C-C4C	3.89	129.86	124.81
24	y	311	CHL	CMD-C2D-C3D	-3.89	118.66	127.61
31	s	415	8CT	C01-C02-C03	-3.89	120.16	124.53
26	2	302	0IE	C23-C16-C15	-3.89	117.47	122.92
24	y	306	CHL	CHC-C1C-NC	3.89	130.10	124.20
24	r	303	CHL	CHA-C4D-ND	3.89	140.63	132.50
24	6	310	CHL	CHD-C4C-C3C	-3.89	119.13	124.84
24	q	309	CHL	CMD-C2D-C3D	-3.89	118.67	127.61
24	s	403	CHL	CHA-C4D-ND	3.89	140.63	132.50
24	5	311	CHL	CHA-C4D-ND	3.88	140.62	132.50
24	9	305	CHL	CHA-C4D-ND	3.88	140.62	132.50
24	s	409	CHL	CHB-C1B-NB	-3.88	120.15	124.26
26	n	302	0IE	C23-C16-C15	-3.88	117.48	122.92
24	y	305	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
24	r	303	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
24	R	602	CHL	CHA-C4D-ND	3.88	140.61	132.50
24	3	309	CHL	CHC-C1C-NC	3.88	130.09	124.20
24	2	318	CHL	C4A-NA-C1A	3.88	108.45	106.71
24	Y	305	CHL	CHC-C1C-NC	3.88	130.08	124.20
24	S	607	CHL	CHB-C1B-NB	-3.87	120.16	124.26
26	Y	303	0IE	C10-C9-C8	3.87	131.41	123.47
26	5	303	0IE	C23-C16-C15	-3.87	117.50	122.92
29	p	301	0UR	C10-C11-C12	-3.87	121.78	127.31
24	1	304	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
31	C	613	8CT	C10-C11-C12	-3.87	120.39	126.23
31	c	613	8CT	C04-C03-C02	-3.87	117.17	122.61
24	s	408	CHL	CMD-C2D-C3D	-3.86	118.72	127.61
26	r	315	0IE	C23-C16-C15	-3.86	117.51	122.92
24	7	310	CHL	C2A-C1A-CHA	-3.86	117.11	123.86
26	6	302	0IE	C10-C9-C8	3.86	131.38	123.47
24	4	317	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
30	N	318	LHG	O7-C7-C8	3.86	119.82	111.50
26	2	303	0IE	C23-C16-C15	-3.86	117.52	122.92
26	R	614	0IE	C23-C16-C15	-3.86	117.52	122.92
24	Y	312	CHL	CHC-C1C-NC	3.86	130.06	124.20
24	1	310	CHL	CMD-C2D-C3D	-3.86	118.74	127.61
26	y	302	0IE	C23-C16-C15	-3.85	117.52	122.92
24	5	305	CHL	CHC-C1C-NC	3.85	130.05	124.20
24	r	308	CHL	C1D-ND-C4D	3.85	109.07	106.33
24	1	305	CHL	CMD-C2D-C3D	-3.85	118.75	127.61
26	G	303	0IE	C20-C3-C4	-3.85	119.88	124.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	308	CHL	C2A-C1A-CHA	-3.85	117.12	123.86
24	u	306	CHL	CHC-C1C-NC	3.85	130.04	124.20
24	7	318	CHL	CMD-C2D-C3D	-3.85	118.76	127.61
24	u	309	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
29	p	301	0UR	C34-C27-C1	-3.85	119.44	124.49
24	p	318	CHL	CMD-C2D-C3D	-3.85	118.76	127.61
24	G	305	CHL	C2A-C1A-CHA	-3.85	117.13	123.86
30	d	407	LHG	O7-C7-C8	3.85	119.79	111.50
24	R	608	CHL	CMD-C2D-C3D	-3.84	118.77	127.61
24	9	312	CHL	C4A-NA-C1A	3.84	108.43	106.71
24	4	310	CHL	CMD-C2D-C3D	-3.84	118.77	127.61
26	Y	302	0IE	C23-C16-C15	-3.84	117.54	122.92
24	y	318	CHL	CMD-C2D-C3D	-3.84	118.78	127.61
24	p	312	CHL	CMD-C2D-C3D	-3.84	118.78	127.61
24	Y	310	CHL	CHC-C1C-NC	3.84	130.03	124.20
26	3	302	0IE	C23-C16-C15	-3.84	117.54	122.92
24	5	312	CHL	CHC-C1C-NC	3.84	130.03	124.20
24	s	414	CHL	CMD-C2D-C3D	-3.84	118.78	127.61
24	9	305	CHL	CMD-C2D-C3D	-3.84	118.78	127.61
24	g	305	CHL	C2A-C1A-CHA	-3.84	117.15	123.86
30	n	318	LHG	O7-C7-C8	3.84	119.77	111.50
32	a	609	SQD	O9-S-O7	-3.84	100.68	113.95
24	G	311	CHL	C2A-C1A-CHA	-3.83	117.15	123.86
24	u	306	CHL	CHA-C4D-ND	3.83	140.52	132.50
26	2	303	0IE	C9-C10-C11	3.83	131.33	123.47
24	N	310	CHL	C2A-C1A-CHA	-3.83	117.16	123.86
29	9	301	0UR	C14-C15-C16	-3.83	121.84	127.31
26	9	302	0IE	C10-C9-C8	3.83	131.32	123.47
26	1	302	0IE	C10-C9-C8	3.83	131.32	123.47
26	4	302	0IE	C23-C16-C15	-3.83	117.56	122.92
24	1	317	CHL	CHD-C4C-C3C	-3.83	119.21	124.84
24	y	305	CHL	C3B-C4B-NB	3.82	114.06	110.52
26	6	302	0IE	C23-C16-C15	-3.82	117.57	122.92
26	p	302	0IE	C23-C16-C15	-3.82	117.57	122.92
26	7	302	0IE	C23-C16-C15	-3.82	117.57	122.92
24	y	313	CHL	CHC-C1C-NC	3.82	130.00	124.20
26	3	302	0IE	C10-C9-C8	3.82	131.30	123.47
24	n	310	CHL	C2A-C1A-CHA	-3.82	117.18	123.86
24	Y	317	CHL	CMD-C2D-C3D	-3.82	118.83	127.61
32	A	609	SQD	O47-C7-C8	3.82	119.73	111.50
24	p	310	CHL	C2A-C1A-CHA	-3.82	117.18	123.86
26	7	302	0IE	C10-C9-C8	3.82	131.30	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	302	0IE	C10-C9-C8	3.82	131.30	123.47
24	Y	317	CHL	CHB-C1B-NB	-3.82	120.22	124.26
24	5	311	CHL	C2A-C1A-CHA	-3.82	117.19	123.86
26	1	302	0IE	C23-C16-C15	-3.81	117.58	122.92
24	y	312	CHL	C1D-ND-C4D	3.81	109.05	106.33
24	8	309	CHL	CHC-C1C-NC	3.81	129.99	124.20
24	R	607	CHL	CHC-C1C-NC	3.81	129.99	124.20
26	N	302	0IE	C23-C16-C15	-3.81	117.58	122.92
29	6	301	0UR	C14-C15-C16	-3.81	121.87	127.31
24	y	318	CHL	CHC-C1C-NC	3.81	129.99	124.20
24	S	613	CHL	CMD-C2D-C3D	-3.81	118.85	127.61
24	2	312	CHL	CHB-C1B-NB	-3.81	120.22	124.26
32	B	618	SQD	O9-S-C6	3.81	111.46	106.94
24	6	305	CHL	CHC-C1C-NC	3.81	129.98	124.20
24	N	312	CHL	CHC-C1C-NC	3.81	129.98	124.20
24	r	308	CHL	CHC-C1C-NC	3.80	129.97	124.20
24	S	607	CHL	CHC-C1C-NC	3.80	129.97	124.20
30	D	407	LHG	O7-C7-C8	3.80	119.69	111.50
24	y	305	CHL	CHC-C1C-NC	3.80	129.97	124.20
24	7	312	CHL	CMD-C2D-C3D	-3.80	118.87	127.61
24	u	306	CHL	CMD-C2D-C3D	-3.80	118.87	127.61
24	2	311	CHL	C2A-C1A-CHA	-3.80	117.22	123.86
24	3	312	CHL	CHD-C4C-C3C	-3.80	119.26	124.84
24	q	310	CHL	C1D-ND-C4D	3.79	109.03	106.33
32	b	618	SQD	O9-S-C6	3.79	111.44	106.94
24	u	311	CHL	C2A-C1A-CHA	-3.79	117.23	123.86
24	2	310	CHL	CMD-C2D-C3D	-3.79	118.90	127.61
24	g	313	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
24	9	308	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
24	q	310	CHL	CHC-C1C-NC	3.79	129.95	124.20
31	S	614	8CT	C01-C02-C03	-3.79	120.28	124.53
24	r	309	CHL	CMD-C2D-C3D	-3.79	118.91	127.61
26	q	302	0IE	C23-C16-C15	-3.78	117.62	122.92
30	A	601	LHG	O7-C7-C8	3.78	119.65	111.50
24	Y	304	CHL	C3B-C4B-NB	3.78	114.02	110.52
24	S	602	CHL	C1D-ND-C4D	3.78	109.02	106.33
24	8	304	CHL	CHC-C1C-NC	3.78	129.94	124.20
24	q	304	CHL	CHC-C1C-NC	3.78	129.94	124.20
26	p	302	0IE	C10-C9-C8	3.78	131.21	123.47
24	r	308	CHL	C3B-C4B-NB	3.78	114.02	110.52
24	9	309	CHL	C2A-C1A-CHA	-3.78	117.25	123.86
26	8	302	0IE	C23-C16-C15	-3.78	117.63	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	408	CHL	CHC-C1C-NC	3.78	129.93	124.20
24	3	305	CHL	CHB-C1B-NB	-3.78	120.26	124.26
24	5	310	CHL	CMD-C2D-C3D	-3.77	118.93	127.61
24	N	309	CHL	C3B-C4B-NB	3.77	114.02	110.52
24	1	305	CHL	CHC-C1C-NC	3.77	129.93	124.20
24	y	312	CHL	CMD-C2D-C3D	-3.77	118.94	127.61
32	a	609	SQD	O47-C7-C8	3.77	119.63	111.50
29	7	301	0UR	C34-C27-C1	-3.77	119.54	124.49
24	Y	311	CHL	CMD-C2D-C3D	-3.77	118.94	127.61
24	y	309	CHL	C2A-C1A-CHA	-3.77	117.27	123.86
26	q	302	0IE	C20-C3-C4	-3.77	119.98	124.83
24	r	308	CHL	CHB-C1B-NB	-3.77	120.27	124.26
24	R	602	CHL	CHC-C1C-NC	3.77	129.92	124.20
24	Y	310	CHL	CMD-C2D-C3D	-3.77	118.95	127.61
24	y	318	CHL	CHB-C1B-NB	-3.77	120.27	124.26
24	2	312	CHL	CHC-C1C-NC	3.76	129.91	124.20
24	q	304	CHL	CAC-C3C-C4C	3.76	129.69	124.81
24	s	403	CHL	C1D-ND-C4D	3.76	109.01	106.33
31	t	101	8CT	C07-C02-C03	-3.76	117.27	122.73
24	S	608	CHL	CHB-C1B-NB	-3.76	120.27	124.26
24	Y	304	CHL	CHC-C1C-NC	3.76	129.91	124.20
24	G	313	CHL	CHD-C4C-C3C	-3.76	119.31	124.84
35	d	403	PHO	C2B-C1B-NB	-3.76	106.93	109.53
24	g	306	CHL	C1D-ND-C4D	3.76	109.00	106.33
24	R	605	CHL	CHC-C1C-NC	3.76	129.90	124.20
24	G	318	CHL	CHC-C1C-NC	3.76	129.90	124.20
26	8	302	0IE	C20-C3-C4	-3.75	120.00	124.83
24	5	306	CHL	CHC-C1C-NC	3.75	129.90	124.20
24	g	311	CHL	C4A-NA-C1A	3.75	108.39	106.71
24	s	403	CHL	CHB-C1B-NB	-3.75	120.28	124.26
35	A	606	PHO	C2B-C1B-NB	-3.75	106.94	109.53
24	Y	317	CHL	CHC-C1C-NC	3.75	129.89	124.20
24	g	306	CHL	CHC-C1C-NC	3.75	129.89	124.20
24	g	318	CHL	CHC-C1C-NC	3.75	129.89	124.20
24	R	606	CHL	CMD-C2D-C3D	-3.74	119.00	127.61
24	R	607	CHL	C3B-C4B-NB	3.74	113.99	110.52
26	g	303	0IE	C20-C3-C4	-3.74	120.01	124.83
24	3	304	CHL	CHC-C1C-NC	3.74	129.88	124.20
24	3	305	CHL	CHC-C1C-NC	3.74	129.88	124.20
24	7	318	CHL	C2A-C1A-CHA	-3.74	117.32	123.85
24	4	305	CHL	CHC-C1C-NC	3.74	129.88	124.20
24	7	312	CHL	CAC-C3C-C4C	3.74	129.66	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	T	101	8CT	C10-C11-C12	-3.74	120.59	126.23
29	1	301	0UR	C9-C8-C7	-3.74	121.98	127.31
24	Y	310	CHL	OBD-CAD-C3D	-3.73	119.54	128.52
26	7	303	0IE	C10-C9-C8	3.73	131.12	123.47
35	D	403	PHO	C2B-C1B-NB	-3.73	106.95	109.53
24	n	312	CHL	CHC-C1C-NC	3.73	129.86	124.20
24	8	304	CHL	CAC-C3C-C4C	3.73	129.65	124.81
24	2	306	CHL	CMD-C2D-C3D	-3.73	119.04	127.61
24	G	309	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
24	9	312	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
24	u	313	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
24	2	306	CHL	CHC-C1C-NC	3.72	129.85	124.20
24	r	303	CHL	CHC-C1C-NC	3.72	129.85	124.20
24	3	317	CHL	C2A-C1A-CHA	-3.72	117.36	123.85
24	r	307	CHL	CMD-C2D-C3D	-3.72	119.06	127.61
24	p	318	CHL	C2A-C1A-CHA	-3.72	117.36	123.85
24	g	311	CHL	C2A-C1A-CHA	-3.72	117.36	123.86
24	2	305	CHL	CHC-C1C-NC	3.71	129.84	124.20
24	n	311	CHL	CHB-C1B-NB	-3.71	120.33	124.26
24	Y	308	CHL	CHC-C1C-NC	3.71	129.83	124.20
24	G	306	CHL	CHC-C1C-NC	3.70	129.82	124.20
31	T	101	8CT	C07-C02-C03	-3.70	117.35	122.73
26	p	303	0IE	C10-C9-C8	3.70	131.06	123.47
24	p	306	CHL	CHD-C4C-NC	3.70	130.04	124.20
32	B	618	SQD	O9-S-O7	-3.70	101.14	113.95
24	y	309	CHL	CHC-C1C-NC	3.70	129.81	124.20
24	u	313	CHL	C4A-NA-C1A	3.70	108.37	106.71
26	g	302	0IE	C10-C9-C8	3.70	131.05	123.47
32	b	618	SQD	O9-S-O7	-3.70	101.16	113.95
24	5	312	CHL	CHB-C1B-NB	-3.70	120.34	124.26
35	a	606	PHO	C2B-C1B-NB	-3.69	106.97	109.53
24	g	309	CHL	CHD-C4C-C3C	-3.69	119.41	124.84
29	6	301	0UR	C5-C4-C3	-3.69	122.56	127.00
24	3	311	CHL	OBD-CAD-C3D	-3.69	119.64	128.52
24	y	310	CHL	C1D-ND-C4D	3.69	108.96	106.33
24	S	608	CHL	C3B-C4B-NB	3.69	113.94	110.52
30	a	601	LHG	O7-C7-C8	3.69	119.45	111.50
24	y	310	CHL	CHC-C1C-NC	3.69	129.80	124.20
24	7	312	CHL	OBD-CAD-C3D	-3.69	119.65	128.52
24	7	306	CHL	CHD-C4C-NC	3.68	130.01	124.20
24	8	309	CHL	C3B-C4B-NB	3.68	113.93	110.52
24	S	613	CHL	CHC-C1C-NC	3.68	129.79	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	CHL	CHC-C1C-NC	3.68	129.79	124.20
24	N	309	CHL	C1D-ND-C4D	3.68	108.95	106.33
32	D	409	SQD	O9-S-O7	-3.68	101.22	113.95
24	7	312	CHL	CHD-C4C-NC	3.68	130.00	124.20
26	u	303	0IE	C20-C3-C4	-3.67	120.10	124.83
24	5	309	CHL	C4A-NA-C1A	3.67	108.36	106.71
24	6	304	CHL	CHC-C1C-NC	3.67	129.78	124.20
24	8	309	CHL	C1D-ND-C4D	3.67	108.94	106.33
29	4	301	0UR	C9-C8-C7	-3.67	122.07	127.31
24	Y	309	CHL	CHC-C1C-NC	3.67	129.77	124.20
31	C	613	8CT	C30-C31-C32	-3.67	116.95	121.47
24	5	306	CHL	CMD-C2D-C3D	-3.67	119.17	127.61
32	b	618	SQD	O5-C5-C4	3.67	116.36	109.69
32	d	409	SQD	O9-S-O7	-3.67	101.25	113.95
26	5	302	0IE	C10-C9-C8	3.67	130.99	123.47
24	7	306	CHL	CMD-C2D-C3D	-3.67	119.18	127.61
24	s	414	CHL	CHC-C1C-NC	3.66	129.76	124.20
24	Y	311	CHL	C1D-ND-C4D	3.66	108.94	106.33
24	N	305	CHL	CHB-C1B-NB	-3.66	120.38	124.26
24	8	310	CHL	CHB-C1B-NB	-3.66	120.38	124.26
24	s	409	CHL	C3B-C4B-NB	3.66	113.91	110.52
31	t	101	8CT	C10-C11-C12	-3.66	120.70	126.23
32	A	609	SQD	O9-S-C6	3.66	111.29	106.94
26	n	302	0IE	C10-C9-C8	3.66	130.97	123.47
32	B	618	SQD	O5-C5-C4	3.66	116.33	109.69
24	9	304	CHL	CHC-C1C-NC	3.65	129.75	124.20
24	9	312	CHL	OBD-CAD-C3D	-3.65	119.74	128.52
24	n	317	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
24	Y	305	CHL	CMD-C2D-C3D	-3.64	119.23	127.61
24	u	318	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
24	R	607	CHL	CHB-C1B-NB	-3.64	120.40	124.26
24	7	313	CHL	CHC-C1C-NC	3.64	129.72	124.20
24	r	306	CHL	CHC-C1C-NC	3.64	129.72	124.20
24	n	311	CHL	CHC-C1C-NC	3.64	129.72	124.20
26	G	302	0IE	C10-C9-C8	3.63	130.92	123.47
24	6	317	CHL	C2A-C1A-CHA	-3.63	117.51	123.85
31	B	617	8CT	C30-C31-C32	-3.63	117.00	121.47
24	8	308	CHL	CHC-C1C-NC	3.63	129.71	124.20
24	n	312	CHL	CAC-C3C-C4C	3.63	129.52	124.81
26	2	302	0IE	C10-C9-C8	3.63	130.91	123.47
26	N	302	0IE	C10-C9-C8	3.63	130.91	123.47
24	Y	305	CHL	C1D-ND-C4D	3.63	108.91	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	609	SQD	O9-S-O7	-3.63	101.39	113.95
24	y	306	CHL	C1D-ND-C4D	3.63	108.91	106.33
24	2	313	CHL	CHC-C1C-NC	3.63	129.71	124.20
24	p	313	CHL	CHC-C1C-NC	3.63	129.71	124.20
24	Y	308	CHL	C2A-C1A-CHA	-3.63	117.52	123.86
24	n	305	CHL	CHB-C1B-NB	-3.63	120.42	124.26
26	p	303	0IE	C20-C3-C4	-3.62	120.17	124.83
24	N	317	CHL	CHD-C4C-C3C	-3.62	119.52	124.84
31	c	613	8CT	C19-C20-C21	-3.62	122.14	127.31
26	R	614	0IE	C10-C9-C8	3.62	130.89	123.47
24	N	312	CHL	CAC-C3C-C4C	3.62	129.51	124.81
24	q	308	CHL	CHC-C1C-NC	3.62	129.69	124.20
24	q	311	CHL	CHB-C1B-NB	-3.61	120.43	124.26
24	q	310	CHL	C3B-C4B-NB	3.61	113.87	110.52
24	9	310	CHL	C2A-C1A-CHA	-3.61	117.54	123.86
32	B	618	SQD	O7-S-C6	3.61	111.23	106.94
24	9	317	CHL	CHD-C4C-C3C	-3.61	119.53	124.84
24	6	305	CHL	CHB-C1B-NB	-3.61	120.44	124.26
24	n	305	CHL	CMD-C2D-C3D	-3.61	119.31	127.61
26	3	303	0IE	C21-C7-C8	-3.61	117.87	122.92
24	r	303	CHL	C1D-ND-C4D	3.61	108.90	106.33
24	p	312	CHL	CHD-C4C-NC	3.61	129.89	124.20
24	p	306	CHL	CMD-C2D-C3D	-3.60	119.32	127.61
24	y	306	CHL	CMD-C2D-C3D	-3.60	119.32	127.61
24	S	602	CHL	CHB-C1B-NB	-3.60	120.44	124.26
24	p	305	CHL	CMB-C2B-C1B	3.60	130.85	125.37
26	9	303	0IE	C21-C7-C8	-3.60	117.89	122.92
24	2	312	CHL	C3B-C4B-NB	3.60	113.85	110.52
24	G	306	CHL	CHB-C1B-NB	-3.60	120.45	124.26
24	p	309	CHL	CHD-C4C-C3C	-3.59	119.56	124.84
28	s	401	NEX	C15-C14-C13	-3.59	122.18	127.31
24	Y	305	CHL	C3B-C4B-NB	3.59	113.85	110.52
24	p	312	CHL	CAC-C3C-C4C	3.59	129.47	124.81
24	g	305	CHL	CHC-C1C-NC	3.59	129.65	124.20
24	5	313	CHL	CHC-C1C-NC	3.59	129.65	124.20
24	9	310	CHL	C4A-NA-C1A	3.59	108.32	106.71
24	R	602	CHL	C1D-ND-C4D	3.59	108.88	106.33
26	q	302	0IE	C9-C10-C11	3.58	130.81	123.47
24	5	310	CHL	CHC-C1C-NC	3.58	129.64	124.20
24	1	311	CHL	C3B-C4B-NB	3.58	113.84	110.52
28	6	303	NEX	C15-C14-C13	-3.58	122.20	127.31
24	N	305	CHL	CMD-C2D-C3D	-3.58	119.38	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	301	0UR	C34-C27-C1	-3.58	119.79	124.49
24	G	305	CHL	CHC-C1C-NC	3.58	129.63	124.20
24	7	310	CHL	CHC-C1C-NC	3.58	129.63	124.20
24	S	602	CHL	CHC-C1C-NC	3.58	129.63	124.20
28	n	303	NEX	C15-C14-C13	-3.58	122.20	127.31
24	5	312	CHL	C3B-C4B-NB	3.58	113.83	110.52
24	6	311	CHL	CHC-C1C-NC	3.58	129.63	124.20
26	N	302	0IE	C4-C3-C2	-3.57	117.01	120.08
24	4	311	CHL	CHC-C1C-NC	3.57	129.62	124.20
24	S	605	CHL	CHC-C1C-NC	3.57	129.62	124.20
24	s	407	CHL	CHC-C1C-NC	3.57	129.62	124.20
32	b	618	SQD	O7-S-C6	3.57	111.18	106.94
24	4	309	CHL	C2A-C1A-CHA	-3.57	117.61	123.86
24	2	310	CHL	CHC-C1C-NC	3.57	129.62	124.20
24	7	306	CHL	C1-C2-C3	-3.57	119.87	126.04
24	S	606	CHL	CHC-C1C-NC	3.57	129.62	124.20
24	3	311	CHL	CHC-C1C-NC	3.57	129.62	124.20
24	u	313	CHL	CHD-C1D-ND	-3.57	121.18	124.45
29	5	301	0UR	C34-C27-C1	-3.57	119.81	124.49
28	N	303	NEX	C15-C14-C13	-3.57	122.22	127.31
24	1	311	CHL	CHB-C1B-NB	-3.57	120.48	124.26
24	y	312	CHL	C3B-C4B-NB	3.57	113.82	110.52
24	s	402	CHL	CAC-C3C-C4C	3.56	129.43	124.81
24	y	306	CHL	C3B-C4B-NB	3.56	113.82	110.52
24	7	305	CHL	CMB-C2B-C1B	3.56	130.79	125.37
24	3	310	CHL	C2A-C1A-CHA	-3.56	117.64	123.86
24	9	304	CHL	C2A-C1A-CHA	-3.56	117.64	123.86
24	6	312	CHL	C2A-C1A-CHA	-3.56	117.64	123.86
29	g	301	0UR	C34-C27-C1	-3.56	119.82	124.49
26	r	315	0IE	C10-C9-C8	3.55	130.76	123.47
24	G	313	CHL	C2A-C1A-CHA	-3.55	117.65	123.86
24	8	310	CHL	CAC-C3C-C4C	3.55	129.42	124.81
26	8	302	0IE	C9-C10-C11	3.55	130.75	123.47
24	s	406	CHL	CHC-C1C-NC	3.55	129.59	124.20
29	2	301	0UR	C34-C27-C1	-3.55	119.84	124.49
24	G	312	CHL	C1-C2-C3	-3.55	121.01	126.75
31	b	617	8CT	C30-C31-C32	-3.55	117.11	121.47
24	Y	309	CHL	CHD-C4C-NC	3.55	129.79	124.20
24	N	311	CHL	CHC-C1C-NC	3.54	129.58	124.20
31	d	410	8CT	C35-C30-C29	-3.54	108.22	112.70
28	r	301	NEX	C15-C14-C13	-3.54	122.26	127.31
31	c	613	8CT	C30-C31-C32	-3.54	117.11	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	306	CHL	C1-C2-C3	-3.54	119.92	126.04
32	a	609	SQD	C44-O6-C1	3.54	120.65	113.74
26	u	303	0IE	C22-C12-C11	-3.54	117.97	122.92
28	3	318	NEX	C15-C14-C13	-3.54	122.26	127.31
29	q	301	0UR	C5-C4-C3	-3.54	122.75	127.00
24	R	605	CHL	CHD-C4C-NC	3.54	129.77	124.20
24	q	311	CHL	CAC-C3C-C4C	3.53	129.40	124.81
24	Y	319	CHL	CHC-C1C-NC	3.53	129.56	124.20
24	s	403	CHL	CAC-C3C-C4C	3.53	129.39	124.81
26	5	302	0IE	C20-C3-C4	-3.53	120.29	124.83
24	8	308	CHL	CAC-C3C-C4C	3.53	129.39	124.81
24	p	312	CHL	C3B-C4B-NB	3.53	113.79	110.52
24	s	402	CHL	OBD-CAD-C3D	-3.53	120.02	128.52
24	S	602	CHL	C3B-C4B-NB	3.53	113.79	110.52
24	u	311	CHL	C4A-NA-C1A	3.53	108.29	106.71
26	2	302	0IE	C20-C3-C4	-3.53	120.29	124.83
24	u	310	CHL	C2A-C1A-CHA	-3.53	117.69	123.86
24	S	607	CHL	C3B-C4B-NB	3.53	113.79	110.52
24	q	308	CHL	CAC-C3C-C4C	3.53	129.39	124.81
24	G	311	CHL	CHC-C1C-NC	3.53	129.55	124.20
24	S	608	CHL	CAC-C3C-C4C	3.52	129.38	124.81
26	3	303	0IE	C6-C7-C8	3.52	124.35	118.94
29	u	301	0UR	C34-C27-C1	-3.52	119.87	124.49
24	3	312	CHL	C2A-C1A-CHA	-3.52	117.70	123.86
24	7	312	CHL	C3B-C4B-NB	3.52	113.78	110.52
24	9	311	CHL	OBD-CAD-C3D	-3.52	120.05	128.52
24	r	307	CHL	CHC-C1C-NC	3.52	129.54	124.20
24	6	304	CHL	C2A-C1A-CHA	-3.52	117.71	123.86
29	y	301	0UR	C9-C8-C7	-3.51	122.29	127.31
24	g	313	CHL	C2A-C1A-CHA	-3.51	117.71	123.86
24	6	311	CHL	OBD-CAD-C3D	-3.51	120.06	128.52
24	p	312	CHL	OBD-CAD-C3D	-3.51	120.06	128.52
24	g	306	CHL	C3B-C4B-NB	3.51	113.77	110.52
24	R	605	CHL	C1D-ND-C4D	3.51	108.83	106.33
24	p	310	CHL	CHC-C1C-NC	3.51	129.53	124.20
24	8	307	CHL	CHC-C1C-NC	3.51	129.53	124.20
24	s	403	CHL	CHC-C1C-NC	3.51	129.53	124.20
24	u	313	CHL	C2A-C1A-CHA	-3.51	117.73	123.86
24	R	608	CHL	CHC-C1C-NC	3.51	129.52	124.20
24	7	312	CHL	C1D-ND-C4D	3.51	108.83	106.33
29	q	301	0UR	C34-C27-C1	-3.51	119.89	124.49
24	R	606	CHL	CHC-C1C-NC	3.51	129.52	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	312	CHL	C2A-C1A-CHA	-3.51	117.73	123.86
31	C	613	8CT	C19-C20-C21	-3.51	122.31	127.31
26	4	302	0IE	C20-C3-C4	-3.51	120.32	124.83
24	N	309	CHL	CHB-C1B-NB	-3.50	120.55	124.26
24	S	602	CHL	CAC-C3C-C4C	3.50	129.36	124.81
24	r	309	CHL	CHC-C1C-NC	3.50	129.52	124.20
24	S	601	CHL	OBD-CAD-C3D	-3.50	120.09	128.52
24	Y	311	CHL	CHD-C4C-NC	3.50	129.72	124.20
24	1	312	CHL	CHC-C1C-NC	3.50	129.52	124.20
24	g	312	CHL	CHC-C1C-NC	3.50	129.52	124.20
24	y	313	CHL	CHB-C1B-NB	-3.50	120.55	124.26
24	Y	310	CHL	CHB-C1B-NB	-3.50	120.55	124.26
24	r	303	CHL	C3B-C4B-NB	3.50	113.76	110.52
24	7	305	CHL	CHD-C4C-NC	3.50	129.71	124.20
24	y	310	CHL	CHD-C4C-NC	3.50	129.71	124.20
24	r	302	CHL	CHC-C1C-NC	3.50	129.51	124.20
24	S	601	CHL	CAC-C3C-C4C	3.50	129.35	124.81
24	N	309	CHL	CAC-C3C-C4C	3.49	129.34	124.81
24	9	312	CHL	CAC-C3C-C4C	3.49	129.34	124.81
24	p	305	CHL	CAC-C3C-C4C	3.49	129.34	124.81
31	S	615	8CT	C10-C11-C12	-3.49	120.97	126.23
24	5	306	CHL	CAC-C3C-C4C	3.49	129.34	124.81
29	Y	301	0UR	C9-C8-C7	-3.49	122.33	127.31
24	g	313	CHL	CHD-C1D-ND	-3.49	121.25	124.45
24	2	306	CHL	CAC-C3C-C4C	3.49	129.33	124.81
24	Y	312	CHL	CAC-C3C-C4C	3.48	129.33	124.81
24	n	309	CHL	CAC-C3C-C4C	3.48	129.33	124.81
24	g	311	CHL	CHC-C1C-NC	3.48	129.49	124.20
26	9	303	0IE	C9-C10-C11	3.48	130.61	123.47
24	s	409	CHL	CAC-C3C-C4C	3.48	129.33	124.81
24	u	313	CHL	OBD-CAD-C3D	-3.48	120.14	128.52
24	g	312	CHL	C1-C2-C3	-3.48	121.12	126.75
29	8	301	0UR	C34-C27-C1	-3.48	119.92	124.49
24	Y	311	CHL	C3B-C4B-NB	3.48	113.74	110.52
24	4	311	CHL	C3B-C4B-NB	3.48	113.74	110.52
24	R	602	CHL	C3B-C4B-NB	3.48	113.74	110.52
24	Y	304	CHL	CHD-C4C-NC	3.48	129.68	124.20
24	2	309	CHL	C4A-NA-C1A	3.48	108.27	106.71
26	1	302	0IE	C20-C3-C4	-3.48	120.36	124.83
24	R	601	CHL	CHC-C1C-NC	3.47	129.47	124.20
24	n	305	CHL	CHC-C1C-NC	3.47	129.47	124.20
24	p	318	CHL	CHC-C1C-NC	3.47	129.47	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	305	CHL	CHD-C4C-NC	3.47	129.68	124.20
24	S	607	CHL	CAC-C3C-C4C	3.47	129.31	124.81
24	q	310	CHL	CHB-C1B-NB	-3.47	120.58	124.26
24	n	311	CHL	C3B-C4B-NB	3.47	113.73	110.52
24	y	310	CHL	CAC-C3C-C4C	3.47	129.31	124.81
24	3	317	CHL	CHC-C1C-NC	3.47	129.46	124.20
24	p	312	CHL	C1D-ND-C4D	3.47	108.80	106.33
24	9	305	CHL	CAC-C3C-C4C	3.46	129.31	124.81
31	D	410	8CT	C35-C30-C29	-3.46	108.32	112.70
32	A	609	SQD	O7-S-C6	3.46	111.06	106.94
24	p	305	CHL	CHD-C4C-NC	3.46	129.66	124.20
24	q	311	CHL	C3B-C4B-NB	3.46	113.73	110.52
24	8	308	CHL	CHB-C1B-NB	-3.46	120.59	124.26
24	u	313	CHL	CAC-C3C-C4C	3.46	129.30	124.81
26	9	303	0IE	C6-C7-C8	3.46	124.25	118.94
24	u	310	CHL	C4A-NA-C1A	3.46	108.26	106.71
24	R	605	CHL	CAC-C3C-C4C	3.46	129.30	124.81
26	u	303	0IE	C10-C9-C8	3.46	130.56	123.47
31	b	617	8CT	C10-C11-C12	-3.46	121.01	126.23
24	q	303	CHL	CHC-C1C-NC	3.46	129.45	124.20
24	1	309	CHL	C2A-C1A-CHA	-3.45	117.82	123.86
24	q	309	CHL	CHC-C1C-NC	3.45	129.44	124.20
24	y	312	CHL	C1-C2-C3	-3.45	121.16	126.75
24	u	306	CHL	CAC-C3C-C4C	3.45	129.29	124.81
26	G	303	0IE	C21-C7-C8	-3.45	118.09	122.92
24	6	305	CHL	CAC-C3C-C4C	3.45	129.29	124.81
24	y	313	CHL	CAC-C3C-C4C	3.45	129.29	124.81
31	b	617	8CT	C01-C02-C07	3.45	120.25	113.62
24	4	312	CHL	CHC-C1C-NC	3.45	129.44	124.20
24	y	312	CHL	CHD-C4C-NC	3.45	129.64	124.20
26	g	303	0IE	C21-C7-C8	-3.45	118.09	122.92
24	Y	317	CHL	CAC-C3C-C4C	3.45	129.28	124.81
24	q	316	CHL	CAA-C2A-C3A	-3.45	108.06	116.10
24	N	305	CHL	CHC-C1C-NC	3.45	129.43	124.20
24	u	305	CHL	CHC-C1C-NC	3.44	129.43	124.20
26	Y	302	0IE	C20-C3-C4	-3.44	120.40	124.83
24	3	309	CHL	C1-C2-C3	-3.44	121.18	126.75
24	1	305	CHL	C3B-C4B-NB	3.44	113.71	110.52
24	y	311	CHL	CHB-C1B-NB	-3.44	120.61	124.26
31	A	608	8CT	C18-C19-C20	-3.44	116.43	123.47
24	Y	304	CHL	OBD-CAD-C3D	-3.44	120.24	128.52
24	n	311	CHL	CHD-C4C-NC	3.44	129.62	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	u	305	CHL	C4A-NA-C1A	3.44	108.25	106.71
24	7	309	CHL	CHD-C4C-C3C	-3.44	119.79	124.84
24	9	312	CHL	CHD-C1D-ND	-3.44	121.30	124.45
24	G	306	CHL	CAC-C3C-C4C	3.44	129.27	124.81
24	n	309	CHL	C1D-ND-C4D	3.43	108.78	106.33
26	u	303	0IE	C21-C7-C8	-3.43	118.11	122.92
24	g	306	CHL	CAC-C3C-C4C	3.43	129.27	124.81
24	s	408	CHL	CAC-C3C-C4C	3.43	129.27	124.81
24	q	308	CHL	CHB-C1B-NB	-3.43	120.62	124.26
24	Y	304	CHL	CAC-C3C-C4C	3.43	129.26	124.81
24	4	312	CHL	CAC-C3C-C4C	3.43	129.26	124.81
24	y	305	CHL	C1D-ND-C4D	3.43	108.77	106.33
24	Y	305	CHL	CHD-C4C-NC	3.43	129.61	124.20
24	s	408	CHL	C3B-C4B-NB	3.43	113.70	110.52
29	4	301	0UR	C34-C27-C1	-3.43	119.99	124.49
26	u	302	0IE	C9-C10-C11	3.43	130.50	123.47
29	n	301	0UR	C14-C15-C16	-3.43	122.42	127.31
24	Y	305	CHL	CHB-C1B-NB	-3.43	120.63	124.26
26	y	302	0IE	C20-C3-C4	-3.43	120.42	124.83
24	9	317	CHL	CHD-C1D-ND	-3.43	121.30	124.45
29	9	301	0UR	C34-C27-C1	-3.43	119.99	124.49
29	Y	301	0UR	O44-C45-C46	3.43	120.67	111.55
24	Y	309	CHL	C1D-ND-C4D	3.43	108.77	106.33
24	3	312	CHL	CHC-C1C-NC	3.43	129.40	124.20
24	Y	309	CHL	CAC-C3C-C4C	3.43	129.26	124.81
24	S	605	CHL	CAC-C3C-C4C	3.43	129.25	124.81
24	p	310	CHL	CAC-C3C-C4C	3.43	129.25	124.81
24	Y	312	CHL	CHB-C1B-NB	-3.42	120.63	124.26
24	3	310	CHL	C4A-NA-C1A	3.42	108.25	106.71
31	s	416	8CT	C25-C24-C23	-3.42	112.54	123.22
29	6	301	0UR	C29-C30-C31	-3.42	107.85	111.74
24	y	306	CHL	C1-C2-C3	-3.42	120.13	126.04
24	1	312	CHL	CAC-C3C-C4C	3.42	129.25	124.81
26	p	303	0IE	C21-C7-C8	-3.42	118.14	122.92
24	y	305	CHL	OBD-CAD-C3D	-3.42	120.30	128.52
24	7	310	CHL	CAC-C3C-C4C	3.42	129.24	124.81
25	c	601	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
24	7	318	CHL	CHC-C1C-NC	3.41	129.38	124.20
24	8	310	CHL	C3B-C4B-NB	3.41	113.68	110.52
31	S	615	8CT	C25-C24-C23	-3.41	112.57	123.22
24	p	305	CHL	C1D-ND-C4D	3.41	108.76	106.33
24	6	310	CHL	C4A-NA-C1A	3.41	108.24	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	304	CHL	C4A-NA-C1A	3.41	108.24	106.71
29	y	301	0UR	O44-C45-C46	3.41	120.62	111.55
24	3	304	CHL	C3B-C4B-NB	3.41	113.68	110.52
24	q	307	CHL	CHC-C1C-NC	3.41	129.37	124.20
25	C	601	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
29	8	301	0UR	C5-C4-C3	-3.41	122.91	127.00
24	5	305	CHL	CAC-C3C-C4C	3.41	129.23	124.81
31	a	608	8CT	C18-C19-C20	-3.40	116.50	123.47
33	m	101	LMG	C8-O7-C10	-3.40	109.41	117.79
24	y	311	CHL	C3B-C4B-NB	3.40	113.67	110.52
24	3	312	CHL	CHD-C1D-ND	-3.40	121.33	124.45
29	1	301	0UR	C34-C27-C1	-3.40	120.03	124.49
24	y	318	CHL	CAC-C3C-C4C	3.40	129.22	124.81
24	6	312	CHL	CHC-C1C-NC	3.40	129.36	124.20
24	y	306	CHL	CHD-C4C-NC	3.40	129.56	124.20
24	G	312	CHL	CHC-C1C-NC	3.40	129.36	124.20
24	3	305	CHL	CAC-C3C-C4C	3.40	129.22	124.81
24	5	313	CHL	CAC-C3C-C4C	3.39	129.21	124.81
24	s	406	CHL	CAC-C3C-C4C	3.39	129.21	124.81
24	Y	311	CHL	C1-C2-C3	-3.39	121.26	126.75
24	N	310	CHL	C4A-NA-C1A	3.39	108.23	106.71
31	B	617	8CT	C01-C02-C07	3.39	120.13	113.62
32	a	609	SQD	O9-S-C6	3.39	110.97	106.94
24	s	403	CHL	C3B-C4B-NB	3.39	113.66	110.52
26	7	303	0IE	C21-C7-C8	-3.39	118.17	122.92
24	6	309	CHL	C1-C2-C3	-3.39	121.27	126.75
24	7	313	CHL	C3B-C4B-NB	3.39	113.66	110.52
24	p	305	CHL	CHB-C1B-NB	-3.39	120.67	124.26
24	2	310	CHL	CAC-C3C-C4C	3.38	129.20	124.81
24	N	312	CHL	C3B-C4B-NB	3.38	113.66	110.52
29	N	301	0UR	C14-C15-C16	-3.38	122.48	127.31
24	G	310	CHL	CAC-C3C-C4C	3.38	129.20	124.81
24	N	311	CHL	CHD-C4C-NC	3.38	129.53	124.20
24	7	305	CHL	CAC-C3C-C4C	3.38	129.20	124.81
24	6	317	CHL	CHC-C1C-NC	3.38	129.33	124.20
24	s	408	CHL	CHD-C4C-NC	3.38	129.53	124.20
24	7	305	CHL	C1D-ND-C4D	3.38	108.74	106.33
29	n	301	0UR	C34-C27-C1	-3.38	120.06	124.49
24	6	312	CHL	C4A-NA-C1A	3.38	108.22	106.71
31	B	617	8CT	C10-C11-C12	-3.38	121.13	126.23
24	g	313	CHL	C4A-NA-C1A	3.37	108.22	106.71
24	8	307	CHL	C2A-C1A-CHA	-3.37	117.96	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	311	CHL	CHC-C1C-NC	3.37	129.32	124.20
24	R	607	CHL	OBD-CAD-C3D	-3.37	120.40	128.52
24	Y	304	CHL	C1D-ND-C4D	3.37	108.73	106.33
24	6	310	CHL	C2A-C1A-CHA	-3.37	117.96	123.86
24	8	303	CHL	CHC-C1C-NC	3.37	129.32	124.20
24	y	306	CHL	CHB-C1B-NB	-3.37	120.69	124.26
24	6	311	CHL	C3B-C4B-NB	3.37	113.64	110.52
24	2	313	CHL	CAC-C3C-C4C	3.37	129.18	124.81
26	r	315	0IE	C9-C10-C11	3.37	130.38	123.47
24	Y	304	CHL	CMB-C2B-C1B	3.37	130.50	125.37
31	C	614	8CT	C01-C02-C07	3.37	120.09	113.62
31	S	614	8CT	C40-C12-C11	3.37	123.38	118.08
24	S	602	CHL	CHD-C4C-NC	3.37	129.51	124.20
24	Y	317	CHL	CHD-C4C-NC	3.37	129.51	124.20
24	n	310	CHL	C4A-NA-C1A	3.37	108.22	106.71
24	r	306	CHL	CAC-C3C-C4C	3.36	129.18	124.81
35	d	403	PHO	CMB-C2B-C3B	3.36	130.97	124.68
24	5	310	CHL	CAC-C3C-C4C	3.36	129.17	124.81
26	9	303	0IE	C22-C12-C11	-3.36	118.21	122.92
24	g	310	CHL	CAC-C3C-C4C	3.36	129.17	124.81
24	R	605	CHL	C3B-C4B-NB	3.36	113.63	110.52
24	y	305	CHL	CAC-C3C-C4C	3.36	129.17	124.81
24	p	311	CHL	CHC-C1C-NC	3.36	129.30	124.20
24	p	313	CHL	C3B-C4B-NB	3.36	113.63	110.52
24	p	306	CHL	C1D-CHD-C4C	-3.36	118.81	126.06
24	4	305	CHL	C3B-C4B-NB	3.36	113.63	110.52
28	s	401	NEX	C24-C23-C22	-3.36	104.29	110.77
24	4	310	CHL	CHC-C1C-NC	3.35	129.29	124.20
24	y	312	CHL	CHB-C1B-NB	-3.35	120.71	124.26
31	c	614	8CT	C01-C02-C07	3.35	120.06	113.62
24	s	403	CHL	CHD-C4C-NC	3.35	129.49	124.20
24	6	310	CHL	CAC-C3C-C4C	3.35	129.16	124.81
24	u	318	CHL	CHD-C1D-ND	-3.35	121.37	124.45
28	r	301	NEX	C24-C23-C22	-3.35	104.30	110.77
24	8	303	CHL	CAC-C3C-C4C	3.35	129.16	124.81
24	s	414	CHL	CHD-C4C-NC	3.35	129.48	124.20
24	3	312	CHL	C4A-NA-C1A	3.35	108.21	106.71
24	u	312	CHL	OBD-CAD-C3D	-3.35	120.46	128.52
24	2	305	CHL	CAC-C3C-C4C	3.35	129.15	124.81
24	p	306	CHL	C1D-ND-C4D	3.35	108.71	106.33
24	q	303	CHL	CAC-C3C-C4C	3.35	129.15	124.81
24	N	311	CHL	C3B-C4B-NB	3.35	113.62	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	318	CHL	CAC-C3C-C4C	3.35	129.15	124.81
24	Y	312	CHL	C3B-C4B-NB	3.35	113.62	110.52
24	u	312	CHL	CAC-C3C-C4C	3.35	129.15	124.81
31	s	415	8CT	C40-C12-C11	3.35	123.35	118.08
24	N	304	CHL	CHC-C1C-NC	3.35	129.28	124.20
28	N	303	NEX	C24-C23-C22	-3.35	104.31	110.77
24	7	309	CHL	CHD-C1D-ND	-3.34	121.38	124.45
24	g	310	CHL	CHC-C1C-NC	3.34	129.28	124.20
26	p	303	0IE	C22-C12-C11	-3.34	118.24	122.92
28	6	303	NEX	C24-C23-C22	-3.34	104.32	110.77
24	Y	305	CHL	C1-C2-C3	-3.34	120.26	126.04
26	n	302	0IE	C4-C3-C2	-3.34	117.21	120.08
24	n	309	CHL	CHD-C4C-NC	3.34	129.47	124.20
28	3	318	NEX	C24-C23-C22	-3.34	104.32	110.77
24	1	310	CHL	CHC-C1C-NC	3.34	129.27	124.20
24	3	308	CHL	CAC-C3C-C4C	3.34	129.15	124.81
24	r	303	CHL	CAC-C3C-C4C	3.34	129.15	124.81
26	y	302	0IE	C9-C10-C11	3.34	130.32	123.47
24	y	310	CHL	C3B-C4B-NB	3.34	113.61	110.52
24	p	306	CHL	C3B-C4B-NB	3.34	113.61	110.52
24	g	318	CHL	CAC-C3C-C4C	3.34	129.14	124.81
24	7	313	CHL	CAC-C3C-C4C	3.34	129.14	124.81
26	G	302	0IE	C21-C7-C8	-3.34	118.25	122.92
24	y	318	CHL	CHD-C4C-NC	3.34	129.47	124.20
28	n	303	NEX	C24-C23-C22	-3.34	104.33	110.77
24	G	310	CHL	CHC-C1C-NC	3.34	129.27	124.20
24	G	309	CHL	CHD-C1D-ND	-3.34	121.39	124.45
24	7	305	CHL	CHB-C1B-NB	-3.34	120.72	124.26
24	S	613	CHL	CHD-C4C-NC	3.34	129.46	124.20
29	3	301	0UR	C14-C15-C16	-3.34	122.55	127.31
26	Y	302	0IE	C9-C10-C11	3.34	130.31	123.47
24	8	315	CHL	CAA-C2A-C3A	-3.34	108.31	116.10
24	R	607	CHL	CHD-C4C-NC	3.34	129.46	124.20
24	5	306	CHL	CHD-C4C-NC	3.34	129.46	124.20
24	r	308	CHL	CHD-C4C-NC	3.34	129.46	124.20
24	7	306	CHL	C1D-ND-C4D	3.33	108.70	106.33
26	4	302	0IE	C21-C7-C8	-3.33	118.25	122.92
24	r	309	CHL	OBD-CAD-C3D	-3.33	120.50	128.52
24	n	312	CHL	C3B-C4B-NB	3.33	113.61	110.52
24	R	608	CHL	C3B-C4B-NB	3.33	113.61	110.52
24	8	309	CHL	CHD-C4C-NC	3.33	129.45	124.20
24	Y	310	CHL	C3B-C4B-NB	3.33	113.61	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	305	CHL	CMB-C2B-C1B	3.33	130.44	125.37
24	p	309	CHL	CHD-C1D-ND	-3.33	121.39	124.45
24	9	312	CHL	C1D-CHD-C4C	-3.33	118.88	126.06
24	y	310	CHL	C1D-CHD-C4C	-3.33	118.88	126.06
24	q	310	CHL	CHD-C4C-NC	3.33	129.45	124.20
26	1	302	0IE	C21-C7-C8	-3.33	118.26	122.92
24	R	602	CHL	CHD-C4C-NC	3.33	129.44	124.20
24	Y	311	CHL	CHB-C1B-NB	-3.33	120.74	124.26
24	3	312	CHL	CAC-C3C-C4C	3.33	129.12	124.81
24	Y	310	CHL	CHD-C4C-NC	3.32	129.44	124.20
24	3	310	CHL	CAC-C3C-C4C	3.32	129.12	124.81
24	5	306	CHL	C3B-C4B-NB	3.32	113.60	110.52
24	g	311	CHL	CAC-C3C-C4C	3.32	129.12	124.81
31	a	608	8CT	C07-C02-C03	-3.32	117.91	122.73
26	p	302	0IE	C21-C7-C8	-3.32	118.27	122.92
31	b	617	8CT	C14-C15-C16	-3.32	117.09	126.42
24	6	308	CHL	CAC-C3C-C4C	3.32	129.12	124.81
24	G	313	CHL	CHD-C1D-ND	-3.32	121.40	124.45
31	b	617	8CT	C07-C02-C03	-3.32	117.91	122.73
25	c	616	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
24	u	318	CHL	CAC-C3C-C4C	3.32	129.11	124.81
24	Y	309	CHL	C1D-CHD-C4C	-3.32	118.90	126.06
26	g	302	0IE	C21-C7-C8	-3.32	118.28	122.92
25	D	405	CLA	O2D-CGD-O1D	-3.32	117.36	123.84
25	C	616	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	1	305	CHL	CHD-C4C-NC	3.31	129.43	124.20
24	s	403	CHL	C1D-CHD-C4C	-3.31	118.91	126.06
24	4	305	CHL	CHD-C4C-NC	3.31	129.42	124.20
24	S	602	CHL	C1D-CHD-C4C	-3.31	118.91	126.06
24	5	305	CHL	C3B-C4B-NB	3.31	113.59	110.52
24	r	309	CHL	C1D-CHD-C4C	-3.31	118.91	126.06
24	G	306	CHL	C3B-C4B-NB	3.31	113.59	110.52
24	9	317	CHL	CAC-C3C-C4C	3.31	129.11	124.81
24	p	313	CHL	CAC-C3C-C4C	3.31	129.11	124.81
24	5	312	CHL	OBD-CAD-C3D	-3.31	120.55	128.52
24	g	313	CHL	CAC-C3C-C4C	3.31	129.10	124.81
24	9	311	CHL	C2A-C1A-CHA	-3.31	118.07	123.86
24	g	306	CHL	CHB-C1B-NB	-3.31	120.75	124.26
24	7	306	CHL	C1D-CHD-C4C	-3.31	118.92	126.06
24	r	303	CHL	CHD-C4C-NC	3.31	129.41	124.20
24	u	312	CHL	C4A-NA-C1A	3.31	108.19	106.71
24	y	313	CHL	C3B-C4B-NB	3.31	113.58	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	305	CHL	C1D-CHD-C4C	-3.31	118.92	126.06
24	u	310	CHL	CHC-C1C-NC	3.31	129.22	124.20
24	n	304	CHL	CHC-C1C-NC	3.31	129.22	124.20
31	x	601	8CT	C07-C02-C03	-3.31	117.93	122.73
24	Y	309	CHL	C3B-C4B-NB	3.31	113.58	110.52
24	y	312	CHL	OBD-CAD-C3D	-3.31	120.56	128.52
25	C	609	CLA	C3B-C4B-NB	-3.30	107.45	110.52
24	R	602	CHL	CAC-C3C-C4C	3.30	129.10	124.81
24	n	305	CHL	C1D-CHD-C4C	-3.30	118.93	126.06
29	N	301	0UR	C34-C27-C1	-3.30	120.15	124.49
24	5	311	CHL	CAC-C3C-C4C	3.30	129.10	124.81
26	u	303	0IE	C13-C12-C11	3.30	124.01	118.94
24	5	310	CHL	CHD-C4C-NC	3.30	129.41	124.20
35	D	403	PHO	CMB-C2B-C3B	3.30	130.86	124.68
24	G	313	CHL	CAC-C3C-C4C	3.30	129.09	124.81
31	c	615	8CT	C19-C18-C17	-3.30	116.71	123.47
24	r	308	CHL	OBD-CAD-C3D	-3.30	120.58	128.52
24	Y	304	CHL	C1-C2-C3	-3.30	120.34	126.04
24	2	310	CHL	CHD-C4C-NC	3.30	129.40	124.20
24	8	308	CHL	CHD-C4C-NC	3.30	129.40	124.20
24	N	310	CHL	C6-C5-C3	-3.30	109.22	114.62
24	R	606	CHL	C3B-C4B-NB	3.30	113.58	110.52
24	S	601	CHL	CHD-C4C-NC	3.30	129.40	124.20
24	R	608	CHL	OBD-CAD-C3D	-3.30	120.58	128.52
31	A	608	8CT	C07-C02-C03	-3.30	117.94	122.73
26	5	302	0IE	C21-C7-C8	-3.30	118.31	122.92
24	9	309	CHL	C4A-NA-C1A	3.30	108.19	106.71
24	G	311	CHL	CAC-C3C-C4C	3.30	129.09	124.81
24	u	310	CHL	CAC-C3C-C4C	3.30	129.09	124.81
24	9	309	CHL	CHC-C1C-NC	3.30	129.20	124.20
24	n	308	CHL	CHC-C1C-NC	3.30	129.20	124.20
24	9	304	CHL	C3B-C4B-NB	3.30	113.57	110.52
24	q	310	CHL	OBD-CAD-C3D	-3.30	120.59	128.52
24	y	318	CHL	C3B-C4B-NB	3.30	113.57	110.52
24	u	313	CHL	CHC-C1C-NC	3.29	129.20	124.20
24	Y	319	CHL	CHD-C4C-NC	3.29	129.39	124.20
24	g	313	CHL	CHC-C1C-NC	3.29	129.20	124.20
25	d	405	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
26	R	614	0IE	C9-C10-C11	3.29	130.22	123.47
24	S	607	CHL	CHD-C4C-NC	3.29	129.39	124.20
26	G	302	0IE	C9-C10-C11	3.29	130.22	123.47
31	a	608	8CT	C30-C31-C32	-3.29	117.42	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	411	LMG	C8-O7-C10	-3.29	109.69	117.79
32	d	409	SQD	O47-C7-C8	3.29	118.59	111.50
31	B	617	8CT	C14-C15-C16	-3.29	117.17	126.42
24	2	306	CHL	CHD-C4C-NC	3.29	129.39	124.20
24	N	308	CHL	CHC-C1C-NC	3.29	129.19	124.20
25	A	607	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
39	D	406	PL9	C7-C3-C2	-3.29	118.98	123.30
24	2	309	CHL	CHC-C1C-NC	3.29	129.19	124.20
26	y	303	0IE	C21-C7-C8	-3.29	118.32	122.92
24	9	308	CHL	CHD-C1D-ND	-3.29	121.44	124.45
26	g	302	0IE	C9-C10-C11	3.28	130.20	123.47
24	8	309	CHL	CHB-C1B-NB	-3.28	120.78	124.26
24	2	311	CHL	CAC-C3C-C4C	3.28	129.07	124.81
26	7	302	0IE	C21-C7-C8	-3.28	118.32	122.92
24	3	304	CHL	CAC-C3C-C4C	3.28	129.07	124.81
24	G	313	CHL	CHC-C1C-NC	3.28	129.18	124.20
24	u	313	CHL	C1D-CHD-C4C	-3.28	118.98	126.06
25	B	609	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
25	a	607	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
24	Y	311	CHL	OBD-CAD-C3D	-3.28	120.62	128.52
24	7	305	CHL	CHB-C4A-NA	3.28	129.05	124.51
24	7	312	CHL	C1D-CHD-C4C	-3.28	118.98	126.06
26	5	303	0IE	C22-C12-C11	-3.28	118.33	122.92
24	s	403	CHL	CMD-C2D-C3D	-3.28	120.07	127.61
31	T	101	8CT	C18-C19-C20	-3.28	116.76	123.47
26	u	302	0IE	C10-C9-C8	3.28	130.19	123.47
24	7	306	CHL	C3B-C4B-NB	3.28	113.56	110.52
24	y	311	CHL	CAC-C3C-C4C	3.28	129.06	124.81
24	1	312	CHL	C1D-CHD-C4C	-3.28	118.99	126.06
24	9	309	CHL	CAC-C3C-C4C	3.28	129.06	124.81
24	4	312	CHL	C1D-CHD-C4C	-3.28	118.99	126.06
24	N	309	CHL	CHD-C4C-NC	3.27	129.36	124.20
31	A	608	8CT	C30-C31-C32	-3.27	117.44	121.47
24	Y	310	CHL	C1D-CHD-C4C	-3.27	119.00	126.06
24	r	303	CHL	CHB-C1B-NB	-3.27	120.79	124.26
24	7	309	CHL	CAC-C3C-C4C	3.27	129.06	124.81
24	n	310	CHL	CHC-C1C-NC	3.27	129.17	124.20
24	q	310	CHL	CAC-C3C-C4C	3.27	129.05	124.81
24	6	312	CHL	CHD-C1D-ND	-3.27	121.45	124.45
24	3	310	CHL	CHC-C1C-NC	3.27	129.16	124.20
26	Y	303	0IE	C21-C7-C8	-3.27	118.34	122.92
24	u	305	CHL	CAC-C3C-C4C	3.27	129.05	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	402	CHL	C1D-CHD-C4C	-3.27	119.01	126.06
25	7	317	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	8	309	CHL	CAC-C3C-C4C	3.27	129.05	124.81
31	B	617	8CT	C07-C02-C03	-3.27	117.99	122.73
24	q	310	CHL	C1D-CHD-C4C	-3.27	119.01	126.06
24	g	310	CHL	CHD-C1D-ND	-3.27	121.45	124.45
24	6	304	CHL	CAC-C3C-C4C	3.27	129.05	124.81
24	6	305	CHL	CHD-C4C-NC	3.27	129.35	124.20
24	n	305	CHL	CHD-C4C-NC	3.27	129.35	124.20
24	p	305	CHL	CHB-C4A-NA	3.26	129.03	124.51
24	6	310	CHL	CHC-C1C-NC	3.26	129.16	124.20
24	Y	310	CHL	CAC-C3C-C4C	3.26	129.04	124.81
25	b	609	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
24	q	308	CHL	CHD-C4C-NC	3.26	129.34	124.20
24	N	310	CHL	CHD-C1D-ND	-3.26	121.46	124.45
24	n	305	CHL	CAC-C3C-C4C	3.26	129.04	124.81
24	R	608	CHL	C1D-CHD-C4C	-3.26	119.02	126.06
26	2	302	0IE	C21-C7-C8	-3.26	118.36	122.92
24	N	305	CHL	CHD-C4C-NC	3.26	129.34	124.20
24	5	312	CHL	CHD-C4C-NC	3.26	129.34	124.20
26	2	303	0IE	C22-C12-C11	-3.26	118.36	122.92
24	y	311	CHL	CHD-C4C-NC	3.26	129.34	124.20
25	D	404	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
24	N	305	CHL	CAC-C3C-C4C	3.26	129.04	124.81
39	d	406	PL9	C7-C3-C2	-3.26	119.01	123.30
24	2	312	CHL	OBD-CAD-C3D	-3.26	120.68	128.52
24	g	305	CHL	C3B-C4B-NB	3.26	113.53	110.52
24	N	310	CHL	CHC-C1C-NC	3.25	129.14	124.20
31	B	617	8CT	C04-C03-C02	-3.25	118.03	122.61
31	C	615	8CT	C24-C23-C21	-3.25	117.27	126.42
31	C	615	8CT	C19-C18-C17	-3.25	116.81	123.47
24	n	310	CHL	CAC-C3C-C4C	3.25	129.03	124.81
24	p	309	CHL	CAC-C3C-C4C	3.25	129.03	124.81
24	S	602	CHL	CMD-C2D-C3D	-3.25	120.13	127.61
24	S	601	CHL	C1D-CHD-C4C	-3.25	119.04	126.06
24	G	310	CHL	CHD-C1D-ND	-3.25	121.47	124.45
24	g	311	CHL	C1D-CHD-C4C	-3.25	119.04	126.06
24	9	312	CHL	CHC-C1C-NC	3.25	129.13	124.20
26	9	302	0IE	C21-C7-C8	-3.25	118.37	122.92
24	Y	319	CHL	C3B-C4B-NB	3.25	113.53	110.52
24	g	306	CHL	CHD-C4C-NC	3.25	129.32	124.20
24	u	312	CHL	C2A-C1A-CHA	-3.25	118.18	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	309	CHL	C1D-CHD-C4C	-3.25	119.05	126.06
24	r	309	CHL	C3B-C4B-NB	3.25	113.53	110.52
31	c	615	8CT	C24-C23-C21	-3.25	117.29	126.42
31	c	614	8CT	C35-C30-C29	-3.25	108.60	112.70
24	N	309	CHL	OBD-CAD-C3D	-3.25	120.71	128.52
24	4	309	CHL	CHC-C1C-NC	3.25	129.13	124.20
24	7	312	CHL	CHB-C1B-NB	-3.25	120.82	124.26
24	u	309	CHL	CHD-C1D-ND	-3.25	121.47	124.45
26	6	302	0IE	C4-C3-C2	-3.25	117.29	120.08
24	6	311	CHL	CHD-C4C-NC	3.24	129.32	124.20
24	g	312	CHL	CAC-C3C-C4C	3.24	129.02	124.81
31	t	101	8CT	C18-C19-C20	-3.24	116.83	123.47
24	g	309	CHL	CHD-C1D-ND	-3.24	121.47	124.45
24	u	311	CHL	CHC-C1C-NC	3.24	129.12	124.20
26	5	303	0IE	C21-C7-C8	-3.24	118.38	122.92
24	q	316	CHL	C1D-CHD-C4C	-3.24	119.06	126.06
25	d	404	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	n	310	CHL	C6-C5-C3	-3.24	109.32	114.62
24	4	308	CHL	CHC-C1C-NC	3.24	129.12	124.20
24	N	310	CHL	CAC-C3C-C4C	3.24	129.01	124.81
24	2	312	CHL	CHD-C4C-NC	3.24	129.31	124.20
24	G	305	CHL	C3B-C4B-NB	3.24	113.52	110.52
24	6	311	CHL	CAC-C3C-C4C	3.24	129.01	124.81
26	3	303	0IE	C22-C12-C11	-3.24	118.39	122.92
24	9	310	CHL	CHD-C1D-ND	-3.24	121.48	124.45
31	b	617	8CT	C04-C03-C02	-3.23	118.06	122.61
24	7	311	CHL	C1D-CHD-C4C	-3.23	119.08	126.06
24	2	311	CHL	CHC-C1C-NC	3.23	129.11	124.20
24	g	312	CHL	OBD-CAD-C3D	-3.23	120.74	128.52
24	r	308	CHL	CAC-C3C-C4C	3.23	129.00	124.81
24	R	607	CHL	CAC-C3C-C4C	3.23	129.00	124.81
26	7	303	0IE	C22-C12-C11	-3.23	118.40	122.92
24	1	308	CHL	CHC-C1C-NC	3.23	129.11	124.20
24	5	318	CHL	CHC-C1C-NC	3.23	129.11	124.20
24	7	311	CHL	CHD-C4C-NC	3.23	129.29	124.20
24	1	310	CHL	CAC-C3C-C4C	3.23	129.00	124.81
24	Y	317	CHL	C3B-C4B-NB	3.23	113.51	110.52
25	c	609	CLA	C3B-C4B-NB	-3.23	107.52	110.52
26	2	303	0IE	C21-C7-C8	-3.23	118.40	122.92
24	1	305	CHL	CAC-C3C-C4C	3.23	129.00	124.81
24	y	309	CHL	CAC-C3C-C4C	3.23	129.00	124.81
24	n	317	CHL	CHD-C1D-ND	-3.23	121.49	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	601	CHL	C4A-NA-C1A	3.23	108.16	106.71
24	1	311	CHL	CHD-C4C-NC	3.23	129.29	124.20
24	y	305	CHL	C1-C2-C3	-3.23	120.46	126.04
24	s	402	CHL	CHD-C4C-NC	3.23	129.29	124.20
24	7	313	CHL	C1D-CHD-C4C	-3.23	119.10	126.06
24	4	311	CHL	CAC-C3C-C4C	3.22	128.99	124.81
31	c	613	8CT	C01-C02-C07	3.22	119.81	113.62
24	2	306	CHL	C3B-C4B-NB	3.22	113.51	110.52
24	Y	305	CHL	C1D-CHD-C4C	-3.22	119.10	126.06
32	D	409	SQD	O47-C7-C8	3.22	118.45	111.50
24	5	311	CHL	CHC-C1C-NC	3.22	129.09	124.20
24	G	312	CHL	CAC-C3C-C4C	3.22	128.99	124.81
24	6	312	CHL	CAC-C3C-C4C	3.22	128.99	124.81
24	3	305	CHL	CHD-C4C-NC	3.22	129.28	124.20
24	9	311	CHL	CAC-C3C-C4C	3.22	128.99	124.81
24	R	602	CHL	CHB-C1B-NB	-3.22	120.85	124.26
27	R	615	XAT	C10-C11-C12	-3.22	113.17	123.22
24	N	317	CHL	CAC-C3C-C4C	3.22	128.99	124.81
25	c	608	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
24	3	311	CHL	C3B-C4B-NB	3.22	113.50	110.52
24	q	303	CHL	C2A-C1A-CHA	-3.22	118.23	123.86
24	S	607	CHL	OBD-CAD-C3D	-3.22	120.78	128.52
26	Y	302	0IE	C10-C9-C8	3.22	130.06	123.47
24	q	307	CHL	C2A-C1A-CHA	-3.22	118.23	123.86
24	R	606	CHL	CHD-C4C-NC	3.22	129.27	124.20
24	N	311	CHL	OBD-CAD-C3D	-3.21	120.78	128.52
24	1	304	CHL	C1D-CHD-C4C	-3.21	119.12	126.06
24	R	601	CHL	CAC-C3C-C4C	3.21	128.98	124.81
24	s	402	CHL	OMC-CMC-C2C	-3.21	118.42	125.69
24	N	317	CHL	CHD-C1D-ND	-3.21	121.50	124.45
24	p	311	CHL	CHD-C4C-NC	3.21	129.26	124.20
31	x	601	8CT	C14-C15-C16	-3.21	117.39	126.42
24	n	308	CHL	C1D-CHD-C4C	-3.21	119.13	126.06
31	s	415	8CT	C39-C16-C15	3.21	123.14	118.08
26	N	302	0IE	C21-C7-C8	-3.21	118.43	122.92
24	1	309	CHL	CHD-C1D-ND	-3.21	121.50	124.45
24	g	312	CHL	C3B-C4B-NB	3.21	113.49	110.52
24	p	313	CHL	C1D-CHD-C4C	-3.21	119.13	126.06
24	S	606	CHL	CAC-C3C-C4C	3.21	128.97	124.81
24	4	305	CHL	CAC-C3C-C4C	3.21	128.97	124.81
32	a	609	SQD	O8-S-C6	3.21	110.85	105.74
24	9	304	CHL	CAC-C3C-C4C	3.21	128.97	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	313	CHL	C4A-NA-C1A	3.21	108.15	106.71
24	u	306	CHL	CHD-C4C-NC	3.21	129.26	124.20
24	s	409	CHL	C1D-CHD-C4C	-3.21	119.14	126.06
26	g	302	0IE	C20-C3-C4	-3.21	120.70	124.83
26	n	302	0IE	C9-C10-C11	3.21	130.04	123.47
24	4	304	CHL	C1D-CHD-C4C	-3.21	119.14	126.06
24	u	311	CHL	CHD-C1D-ND	-3.21	121.51	124.45
24	n	308	CHL	CHD-C1D-ND	-3.20	121.51	124.45
24	g	305	CHL	CAC-C3C-C4C	3.20	128.97	124.81
25	C	608	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
25	p	315	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
24	5	306	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
24	u	306	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
24	q	309	CHL	CHD-C4C-NC	3.20	129.25	124.20
24	G	313	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
24	s	403	CHL	OBD-CAD-C3D	-3.20	120.81	128.52
24	s	406	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
24	N	304	CHL	CAC-C3C-C4C	3.20	128.97	124.81
24	u	311	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
24	3	311	CHL	CAC-C3C-C4C	3.20	128.96	124.81
24	2	318	CHL	CHC-C1C-NC	3.20	129.06	124.20
31	X	601	8CT	C14-C15-C16	-3.20	117.42	126.42
24	3	311	CHL	CHD-C4C-NC	3.20	129.25	124.20
24	8	309	CHL	OBD-CAD-C3D	-3.20	120.82	128.52
24	5	309	CHL	CAC-C3C-C4C	3.20	128.96	124.81
24	4	309	CHL	CHD-C1D-ND	-3.20	121.51	124.45
24	q	311	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
26	6	302	0IE	C21-C7-C8	-3.20	118.44	122.92
26	n	302	0IE	C21-C7-C8	-3.20	118.44	122.92
24	R	601	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	8	310	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	5	318	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	n	304	CHL	CAC-C3C-C4C	3.20	128.96	124.81
24	y	306	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	9	311	CHL	C4A-NA-C1A	3.20	108.14	106.71
24	9	310	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	p	309	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
25	B	607	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
24	9	309	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	y	311	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
24	7	309	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
26	y	302	0IE	C10-C9-C8	3.20	130.02	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	608	CHL	C1D-CHD-C4C	-3.19	119.17	126.06
24	2	318	CHL	C1D-CHD-C4C	-3.19	119.17	126.06
25	7	315	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
24	4	310	CHL	C1D-CHD-C4C	-3.19	119.17	126.06
26	G	303	0IE	C22-C12-C11	-3.19	118.45	122.92
24	5	309	CHL	CHC-C1C-NC	3.19	129.05	124.20
24	p	311	CHL	C1D-CHD-C4C	-3.19	119.17	126.06
24	3	317	CHL	CAC-C3C-C4C	3.19	128.95	124.81
26	u	303	0IE	C6-C7-C8	3.19	123.84	118.94
26	N	302	0IE	C9-C10-C11	3.19	130.01	123.47
24	n	311	CHL	OBD-CAD-C3D	-3.19	120.84	128.52
24	g	306	CHL	C1-C2-C3	-3.19	120.53	126.04
24	2	312	CHL	CAC-C3C-C4C	3.19	128.95	124.81
24	3	311	CHL	C1D-CHD-C4C	-3.19	119.18	126.06
24	u	312	CHL	CHC-C1C-NC	3.19	129.04	124.20
24	Y	308	CHL	CAC-C3C-C4C	3.19	128.94	124.81
24	7	310	CHL	C1D-CHD-C4C	-3.19	119.18	126.06
24	u	318	CHL	C1D-CHD-C4C	-3.19	119.19	126.06
24	9	311	CHL	CHC-C1C-NC	3.18	129.03	124.20
24	8	308	CHL	C1D-CHD-C4C	-3.18	119.19	126.06
24	g	313	CHL	C1D-CHD-C4C	-3.18	119.19	126.06
24	7	309	CHL	CHC-C1C-NC	3.18	129.03	124.20
26	G	302	0IE	C20-C3-C4	-3.18	120.73	124.83
24	9	310	CHL	CHC-C1C-NC	3.18	129.03	124.20
24	s	407	CHL	CAC-C3C-C4C	3.18	128.94	124.81
26	p	303	0IE	C9-C10-C11	3.18	129.99	123.47
24	r	306	CHL	CHD-C4C-NC	3.18	129.22	124.20
24	8	309	CHL	CMB-C2B-C1B	3.18	130.21	125.37
24	r	302	CHL	C4A-NA-C1A	3.18	108.14	106.71
24	9	317	CHL	C1D-CHD-C4C	-3.18	119.20	126.06
26	4	302	0IE	C9-C10-C11	3.18	129.99	123.47
31	D	410	8CT	C05-C04-C03	3.18	115.38	110.48
31	S	614	8CT	C39-C16-C15	3.18	123.09	118.08
26	R	614	0IE	C21-C7-C8	-3.18	118.47	122.92
24	4	311	CHL	OBD-CAD-C3D	-3.18	120.87	128.52
24	s	407	CHL	C1D-CHD-C4C	-3.18	119.20	126.06
24	4	317	CHL	CHC-C1C-NC	3.18	129.02	124.20
24	G	305	CHL	CAC-C3C-C4C	3.18	128.93	124.81
24	4	309	CHL	CAC-C3C-C4C	3.18	128.93	124.81
24	1	310	CHL	C1D-CHD-C4C	-3.18	119.21	126.06
24	9	305	CHL	C1D-CHD-C4C	-3.18	119.21	126.06
24	r	307	CHL	C3B-C4B-NB	3.18	113.46	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	304	CHL	CHD-C1D-ND	-3.18	121.54	124.45
24	6	311	CHL	C1D-CHD-C4C	-3.17	119.21	126.06
24	G	312	CHL	OBD-CAD-C3D	-3.17	120.88	128.52
26	2	303	0IE	C10-C9-C8	3.17	129.98	123.47
24	2	305	CHL	C3B-C4B-NB	3.17	113.46	110.52
24	R	606	CHL	C1D-CHD-C4C	-3.17	119.21	126.06
24	1	317	CHL	CHC-C1C-NC	3.17	129.02	124.20
29	p	301	0UR	C5-C4-C3	-3.17	123.19	127.00
29	q	301	0UR	C43-C3-C4	-3.17	121.18	125.02
24	S	602	CHL	OBD-CAD-C3D	-3.17	120.89	128.52
24	g	312	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
24	S	601	CHL	C3B-C4B-NB	3.17	113.46	110.52
25	b	611	CLA	C1-C2-C3	-3.17	120.56	126.04
26	r	315	0IE	C21-C7-C8	-3.17	118.48	122.92
24	7	311	CHL	CAC-C3C-C4C	3.17	128.92	124.81
24	7	312	CHL	OMC-CMC-C2C	-3.17	118.52	125.69
24	G	318	CHL	CHD-C4C-NC	3.17	129.20	124.20
26	g	302	0IE	C22-C12-C11	-3.17	118.48	122.92
26	1	302	0IE	C9-C10-C11	3.17	129.97	123.47
24	p	310	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
24	q	308	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
24	2	306	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
24	S	606	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
26	g	303	0IE	C22-C12-C11	-3.17	118.48	122.92
24	G	311	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
24	y	313	CHL	OBD-CAD-C3D	-3.17	120.90	128.52
24	8	315	CHL	C1D-CHD-C4C	-3.17	119.23	126.06
24	s	414	CHL	CAC-C3C-C4C	3.16	128.91	124.81
29	3	301	0UR	C5-C4-C3	-3.16	123.20	127.00
24	Y	312	CHL	OBD-CAD-C3D	-3.16	120.91	128.52
24	G	312	CHL	C1D-CHD-C4C	-3.16	119.23	126.06
24	p	318	CHL	CAC-C3C-C4C	3.16	128.91	124.81
24	S	605	CHL	C1D-CHD-C4C	-3.16	119.24	126.06
26	G	302	0IE	C22-C12-C11	-3.16	118.49	122.92
24	q	310	CHL	CMB-C2B-C1B	3.16	130.18	125.37
24	1	309	CHL	CAC-C3C-C4C	3.16	128.91	124.81
24	p	312	CHL	C1D-CHD-C4C	-3.16	119.24	126.06
24	9	317	CHL	CAA-C2A-C3A	-3.16	108.72	116.10
31	d	410	8CT	C05-C04-C03	3.16	115.35	110.48
24	q	309	CHL	C1D-CHD-C4C	-3.16	119.24	126.06
24	1	309	CHL	CHC-C1C-NC	3.16	129.00	124.20
24	1	311	CHL	CAC-C3C-C4C	3.16	128.91	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	304	CHL	CHD-C1D-ND	-3.16	121.55	124.45
24	N	317	CHL	CAA-C2A-C3A	-3.16	108.73	116.10
24	4	310	CHL	CAC-C3C-C4C	3.16	128.91	124.81
24	q	307	CHL	CAC-C3C-C4C	3.16	128.91	124.81
24	g	318	CHL	CHD-C4C-NC	3.16	129.18	124.20
24	S	605	CHL	C3B-C4B-NB	3.16	113.44	110.52
24	N	308	CHL	CHD-C1D-ND	-3.16	121.55	124.45
25	b	607	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
24	1	311	CHL	OBD-CAD-C3D	-3.16	120.92	128.52
29	2	301	0UR	C9-C8-C7	-3.16	122.81	127.31
24	G	306	CHL	C1-C2-C3	-3.16	120.59	126.04
24	9	305	CHL	CHD-C4C-NC	3.15	129.17	124.20
26	3	302	0IE	C21-C7-C8	-3.15	118.51	122.92
26	8	302	0IE	C21-C7-C8	-3.15	118.51	122.92
24	n	317	CHL	CAC-C3C-C4C	3.15	128.90	124.81
31	s	416	8CT	C10-C11-C12	-3.15	121.47	126.23
24	n	317	CHL	CHC-C1C-NC	3.15	128.99	124.20
24	p	309	CHL	CHC-C1C-NC	3.15	128.99	124.20
24	8	304	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
24	4	308	CHL	CHD-C1D-ND	-3.15	121.56	124.45
24	s	414	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
37	c	619	DGD	O1G-C1A-C2A	3.15	121.80	111.91
24	n	317	CHL	CAA-C2A-C3A	-3.15	108.75	116.10
24	4	311	CHL	CHD-C4C-NC	3.15	129.17	124.20
26	9	302	0IE	C4-C3-C2	-3.15	117.38	120.08
24	r	302	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
24	8	303	CHL	C4A-NA-C1A	3.15	108.12	106.71
24	1	308	CHL	CHD-C1D-ND	-3.15	121.56	124.45
24	Y	319	CHL	C1D-CHD-C4C	-3.15	119.27	126.06
24	r	302	CHL	CAC-C3C-C4C	3.15	128.90	124.81
24	R	605	CHL	CHB-C1B-NB	-3.15	120.92	124.26
24	9	310	CHL	OBD-CAD-C3D	-3.15	120.95	128.52
24	Y	310	CHL	O2A-CGA-CBA	3.15	121.78	111.91
24	s	414	CHL	C3B-C4B-NB	3.15	113.43	110.52
24	u	318	CHL	CHC-C1C-NC	3.15	128.97	124.20
24	7	318	CHL	CAC-C3C-C4C	3.15	128.89	124.81
24	q	304	CHL	C1D-CHD-C4C	-3.15	119.27	126.06
39	d	406	PL9	C7-C8-C9	-3.14	121.56	126.79
24	n	309	CHL	CHB-C1B-NB	-3.14	120.93	124.26
29	6	301	0UR	C34-C27-C1	-3.14	120.36	124.49
24	p	306	CHL	CHB-C4A-NA	3.14	128.86	124.51
24	9	317	CHL	CHC-C1C-NC	3.14	128.97	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	313	CHL	C1D-CHD-C4C	-3.14	119.28	126.06
27	r	316	XAT	C10-C11-C12	-3.14	113.41	123.22
24	y	311	CHL	OBD-CAD-C3D	-3.14	120.96	128.52
24	S	613	CHL	CAC-C3C-C4C	3.14	128.89	124.81
24	G	318	CHL	C3B-C4B-NB	3.14	113.43	110.52
24	4	304	CHL	CHC-C1C-NC	3.14	128.97	124.20
39	D	406	PL9	C7-C8-C9	-3.14	121.56	126.79
24	r	307	CHL	C1D-CHD-C4C	-3.14	119.28	126.06
24	n	317	CHL	C1D-CHD-C4C	-3.14	119.28	126.06
31	s	415	8CT	C25-C24-C23	-3.14	113.42	123.22
24	3	304	CHL	CMB-C2B-C1B	3.14	130.15	125.37
24	y	309	CHL	C3B-C4B-NB	3.14	113.42	110.52
24	N	317	CHL	CHC-C1C-NC	3.14	128.96	124.20
25	B	611	CLA	C1-C2-C3	-3.13	120.62	126.04
24	s	408	CHL	C1D-CHD-C4C	-3.13	119.30	126.06
24	G	311	CHL	C4A-NA-C1A	3.13	108.11	106.71
27	r	316	XAT	C24-C23-C22	-3.13	104.72	110.77
24	N	317	CHL	C1D-CHD-C4C	-3.13	119.30	126.06
24	5	312	CHL	CAC-C3C-C4C	3.13	128.88	124.81
24	Y	308	CHL	C3B-C4B-NB	3.13	113.42	110.52
24	4	317	CHL	CHD-C1D-ND	-3.13	121.58	124.45
24	N	312	CHL	C1D-CHD-C4C	-3.13	119.30	126.06
24	Y	312	CHL	C1D-CHD-C4C	-3.13	119.30	126.06
24	2	305	CHL	CHD-C4C-NC	3.13	129.14	124.20
24	p	310	CHL	OBD-CAD-C3D	-3.13	120.99	128.52
24	1	317	CHL	CHD-C1D-ND	-3.13	121.58	124.45
24	p	312	CHL	CHB-C1B-NB	-3.13	120.94	124.26
26	p	303	0IE	C6-C7-C8	3.13	123.74	118.94
24	q	309	CHL	C3B-C4B-NB	3.13	113.42	110.52
24	q	304	CHL	CHD-C4C-NC	3.13	129.13	124.20
24	S	606	CHL	CHD-C4C-NC	3.13	129.13	124.20
29	3	301	0UR	C34-C27-C1	-3.13	120.39	124.49
24	R	602	CHL	C1D-CHD-C4C	-3.13	119.31	126.06
25	2	308	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
24	3	309	CHL	C4A-NA-C1A	3.13	108.11	106.71
24	8	304	CHL	CHD-C4C-NC	3.12	129.13	124.20
24	r	303	CHL	C1D-CHD-C4C	-3.12	119.32	126.06
27	R	615	XAT	C24-C23-C22	-3.12	104.74	110.77
24	G	306	CHL	CHD-C4C-NC	3.12	129.12	124.20
31	d	410	8CT	C01-C02-C07	3.12	119.62	113.62
26	5	303	0IE	C10-C9-C8	3.12	129.87	123.47
24	N	309	CHL	C1D-CHD-C4C	-3.12	119.32	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	315	CHL	CHD-C1D-ND	-3.12	121.58	124.45
24	6	312	CHL	C1D-CHD-C4C	-3.12	119.32	126.06
31	V	401	8CT	C18-C19-C20	-3.12	117.08	123.47
26	n	302	0IE	C20-C3-C4	-3.12	120.81	124.83
24	9	311	CHL	CHD-C4C-NC	3.12	129.12	124.20
24	5	305	CHL	CHD-C4C-NC	3.12	129.12	124.20
25	p	317	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
24	1	304	CHL	CHC-C1C-NC	3.12	128.94	124.20
24	u	309	CHL	CHC-C1C-NC	3.12	128.94	124.20
24	r	307	CHL	CHD-C4C-NC	3.12	129.12	124.20
24	6	317	CHL	CAC-C3C-C4C	3.12	128.86	124.81
24	3	305	CHL	C1D-CHD-C4C	-3.12	119.33	126.06
24	s	407	CHL	CHD-C4C-NC	3.12	129.12	124.20
26	9	302	0IE	C9-C10-C11	3.12	129.86	123.47
24	u	306	CHL	C1-C2-C3	-3.12	120.65	126.04
24	u	318	CHL	CAA-C2A-C3A	-3.12	108.82	116.10
24	8	315	CHL	CAC-C3C-C4C	3.12	128.86	124.81
24	y	305	CHL	CHB-C4A-NA	3.12	128.82	124.51
24	n	312	CHL	C1D-CHD-C4C	-3.12	119.33	126.06
25	R	612	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	S	613	CHL	C1D-CHD-C4C	-3.12	119.33	126.06
24	9	305	CHL	C1-C2-C3	-3.12	120.65	126.04
24	u	312	CHL	C1D-CHD-C4C	-3.12	119.33	126.06
29	8	301	0UR	C43-C3-C4	-3.12	121.25	125.02
24	S	613	CHL	C3B-C4B-NB	3.12	113.41	110.52
24	q	304	CHL	C3B-C4B-NB	3.12	113.41	110.52
24	1	308	CHL	C1D-CHD-C4C	-3.11	119.34	126.06
31	S	614	8CT	C25-C24-C23	-3.11	113.50	123.22
26	y	302	0IE	C22-C12-C11	-3.11	118.56	122.92
24	u	312	CHL	CHD-C4C-NC	3.11	129.11	124.20
24	1	305	CHL	OBD-CAD-C3D	-3.11	121.03	128.52
31	C	614	8CT	C35-C30-C29	-3.11	108.76	112.70
24	q	316	CHL	CHC-C1C-NC	3.11	128.93	124.20
25	S	604	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	G	312	CHL	C3B-C4B-NB	3.11	113.40	110.52
26	y	302	0IE	C21-C7-C8	-3.11	118.56	122.92
24	Y	312	CHL	CHD-C4C-NC	3.11	129.11	124.20
26	Y	302	0IE	C21-C7-C8	-3.11	118.56	122.92
24	3	309	CHL	CHD-C1D-ND	-3.11	121.59	124.45
29	3	301	0UR	C48-C47-C46	-3.11	119.17	125.85
31	v	401	8CT	C18-C19-C20	-3.11	117.10	123.47
24	Y	304	CHL	CHB-C1B-NB	-3.11	120.96	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	604	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	3	308	CHL	CHC-C1C-NC	3.11	128.92	124.20
26	q	302	0IE	C21-C7-C8	-3.11	118.57	122.92
25	B	602	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	3	310	CHL	CHD-C1D-ND	-3.11	121.60	124.45
24	Y	319	CHL	CAC-C3C-C4C	3.11	128.84	124.81
24	u	311	CHL	OBD-CAD-C3D	-3.11	121.04	128.52
24	6	304	CHL	CMB-C2B-C1B	3.11	130.10	125.37
24	G	305	CHL	CHD-C4C-NC	3.11	129.10	124.20
24	6	310	CHL	CHD-C1D-ND	-3.11	121.60	124.45
24	u	310	CHL	C1D-CHD-C4C	-3.11	119.36	126.06
25	5	308	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
29	q	301	0UR	C29-C30-C31	-3.10	108.21	111.74
24	8	303	CHL	C2A-C1A-CHA	-3.10	118.43	123.86
24	6	308	CHL	CHC-C1C-NC	3.10	128.91	124.20
24	s	406	CHL	C3B-C4B-NB	3.10	113.39	110.52
24	R	608	CHL	CHD-C4C-NC	3.10	129.09	124.20
24	7	318	CHL	C1D-CHD-C4C	-3.10	119.36	126.06
24	g	306	CHL	C1D-CHD-C4C	-3.10	119.36	126.06
26	G	303	0IE	C6-C7-C8	3.10	123.70	118.94
24	g	305	CHL	CHD-C4C-NC	3.10	129.09	124.20
24	G	310	CHL	C1D-CHD-C4C	-3.10	119.36	126.06
24	7	310	CHL	OBD-CAD-C3D	-3.10	121.05	128.52
25	6	307	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
24	9	308	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
24	r	309	CHL	CHD-C4C-NC	3.10	129.09	124.20
24	G	306	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
24	1	309	CHL	OBD-CAD-C3D	-3.10	121.06	128.52
24	6	305	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
25	B	604	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	G	318	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
24	q	304	CHL	OBD-CAD-C3D	-3.10	121.06	128.52
24	q	309	CHL	CAC-C3C-C4C	3.10	128.83	124.81
24	4	308	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
26	Y	302	0IE	C22-C12-C11	-3.10	118.58	122.92
24	8	315	CHL	CHC-C1C-NC	3.10	128.90	124.20
29	5	301	0UR	C9-C8-C7	-3.10	122.89	127.31
24	g	318	CHL	C1D-CHD-C4C	-3.10	119.38	126.06
24	3	312	CHL	C1D-CHD-C4C	-3.10	119.38	126.06
24	g	310	CHL	C1D-CHD-C4C	-3.10	119.38	126.06
24	p	306	CHL	CAC-C3C-C4C	3.10	128.83	124.81
31	x	601	8CT	C11-C10-C03	-3.10	118.50	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	305	CHL	CHB-C1B-NB	-3.10	120.98	124.26
24	6	309	CHL	C1D-CHD-C4C	-3.10	119.38	126.06
24	N	304	CHL	C2A-C1A-CHA	-3.10	118.44	123.86
24	9	304	CHL	CMB-C2B-C1B	3.10	130.08	125.37
24	2	306	CHL	CHB-C1B-NB	-3.10	120.98	124.26
25	r	313	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
29	8	301	0UR	C29-C30-C31	-3.10	108.22	111.74
24	1	305	CHL	C1D-CHD-C4C	-3.09	119.38	126.06
24	g	311	CHL	CHD-C1D-ND	-3.09	121.61	124.45
24	5	313	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
24	y	305	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
24	Y	304	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
26	g	303	0IE	C6-C7-C8	3.09	123.69	118.94
25	A	604	CLA	C3B-C4B-NB	-3.09	107.65	110.52
24	5	311	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
24	6	317	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
25	s	405	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
26	2	302	0IE	C22-C12-C11	-3.09	118.59	122.92
24	2	313	CHL	CHD-C1D-ND	-3.09	121.61	124.45
24	2	313	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
29	N	301	0UR	C43-C3-C4	-3.09	121.28	125.02
24	4	309	CHL	OBD-CAD-C3D	-3.09	121.08	128.52
24	p	318	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
24	5	313	CHL	CHD-C1D-ND	-3.09	121.61	124.45
24	4	305	CHL	OBD-CAD-C3D	-3.09	121.09	128.52
24	2	309	CHL	CAC-C3C-C4C	3.09	128.82	124.81
24	Y	311	CHL	C1D-CHD-C4C	-3.09	119.40	126.06
24	5	313	CHL	C3B-C4B-NB	3.09	113.38	110.52
24	9	311	CHL	C1D-CHD-C4C	-3.09	119.40	126.06
24	Y	317	CHL	C1D-CHD-C4C	-3.09	119.40	126.06
24	s	403	CHL	C1-C2-C3	-3.09	120.71	126.04
24	2	313	CHL	C3B-C4B-NB	3.09	113.38	110.52
24	q	316	CHL	CHD-C1D-ND	-3.08	121.62	124.45
24	q	304	CHL	C1-C2-C3	-3.08	120.71	126.04
31	t	101	8CT	C11-C10-C03	-3.08	118.54	127.20
24	8	304	CHL	OBD-CAD-C3D	-3.08	121.10	128.52
24	1	310	CHL	CHD-C4C-NC	3.08	129.06	124.20
25	a	604	CLA	C3B-C4B-NB	-3.08	107.66	110.52
24	n	310	CHL	CHD-C1D-ND	-3.08	121.62	124.45
25	b	602	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
31	B	617	8CT	C11-C10-C03	-3.08	118.55	127.20
24	s	406	CHL	CHD-C4C-NC	3.08	129.06	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	313	CHL	OBD-CAD-C3D	-3.08	121.11	128.52
24	p	305	CHL	OBD-CAD-C3D	-3.08	121.11	128.52
24	G	310	CHL	C4A-NA-C1A	3.08	108.09	106.71
24	9	308	CHL	CHC-C1C-NC	3.08	128.88	124.20
31	b	617	8CT	C11-C10-C03	-3.08	118.55	127.20
29	p	301	0UR	C48-C47-C46	-3.08	119.25	125.85
24	y	313	CHL	CHD-C4C-NC	3.08	129.05	124.20
31	T	101	8CT	C11-C10-C03	-3.08	118.56	127.20
24	G	311	CHL	CHD-C1D-ND	-3.08	121.63	124.45
35	D	403	PHO	O2D-CGD-O1D	-3.08	117.82	123.84
24	n	309	CHL	C1D-CHD-C4C	-3.08	119.42	126.06
24	N	308	CHL	C3B-C4B-NB	3.08	113.37	110.52
31	C	614	8CT	C05-C04-C03	3.08	115.22	110.48
24	G	313	CHL	OBD-CAD-C3D	-3.07	121.12	128.52
26	9	303	0IE	C13-C12-C11	3.07	123.66	118.94
26	7	303	0IE	C6-C7-C8	3.07	123.66	118.94
24	R	606	CHL	CAC-C3C-C4C	3.07	128.80	124.81
24	2	311	CHL	C1D-CHD-C4C	-3.07	119.43	126.06
24	9	305	CHL	CMB-C2B-C1B	3.07	130.05	125.37
29	g	301	0UR	O44-C45-C46	3.07	119.72	111.55
31	X	601	8CT	C11-C10-C03	-3.07	118.57	127.20
24	g	318	CHL	C3B-C4B-NB	3.07	113.36	110.52
24	g	310	CHL	C4A-NA-C1A	3.07	108.09	106.71
24	p	311	CHL	CAC-C3C-C4C	3.07	128.79	124.81
24	8	304	CHL	C3B-C4B-NB	3.07	113.36	110.52
24	y	312	CHL	C1D-CHD-C4C	-3.07	119.43	126.06
35	d	403	PHO	O2D-CGD-O1D	-3.07	117.83	123.84
24	y	311	CHL	O2A-CGA-CBA	3.07	121.54	111.91
24	1	304	CHL	CAC-C3C-C4C	3.07	128.79	124.81
24	9	308	CHL	CAC-C3C-C4C	3.07	128.79	124.81
24	4	310	CHL	CHD-C4C-NC	3.07	129.04	124.20
31	a	608	8CT	C11-C10-C03	-3.07	118.58	127.20
24	2	318	CHL	CAC-C3C-C4C	3.07	128.79	124.81
29	9	301	0UR	C5-C4-C3	-3.07	123.32	127.00
24	Y	310	CHL	CMB-C2B-C1B	3.07	130.04	125.37
24	3	317	CHL	OBD-CAD-C3D	-3.07	121.14	128.52
24	S	605	CHL	CHD-C4C-NC	3.07	129.03	124.20
24	5	310	CHL	C3B-C4B-NB	3.07	113.36	110.52
24	Y	304	CHL	CHB-C4A-NA	3.07	128.75	124.51
24	p	311	CHL	CHD-C1D-ND	-3.07	121.64	124.45
24	3	309	CHL	C1D-CHD-C4C	-3.06	119.45	126.06
29	6	301	0UR	C48-C47-C46	-3.06	119.28	125.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	u	301	0UR	C5-C4-C3	-3.06	123.32	127.00
24	n	310	CHL	C1D-CHD-C4C	-3.06	119.45	126.06
24	7	318	CHL	CHD-C4C-NC	3.06	129.03	124.20
29	G	301	0UR	O44-C45-C46	3.06	119.69	111.55
24	n	312	CHL	CHD-C1D-ND	-3.06	121.64	124.45
24	7	305	CHL	OBD-CAD-C3D	-3.06	121.15	128.52
24	n	312	CHL	OBD-CAD-C3D	-3.06	121.16	128.52
24	5	309	CHL	CMB-C2B-C1B	3.06	130.03	125.37
26	5	302	0IE	C22-C12-C11	-3.06	118.64	122.92
29	2	301	0UR	C48-C47-C46	-3.06	119.29	125.85
24	4	305	CHL	C1D-CHD-C4C	-3.06	119.46	126.06
24	y	318	CHL	C1D-CHD-C4C	-3.06	119.46	126.06
24	7	310	CHL	CHD-C4C-NC	3.06	129.02	124.20
26	3	302	0IE	C22-C12-C11	-3.06	118.64	122.92
24	q	316	CHL	CAC-C3C-C4C	3.06	128.78	124.81
24	7	306	CHL	CHB-C4A-NA	3.06	128.74	124.51
24	2	306	CHL	OBD-CAD-C3D	-3.06	121.16	128.52
24	9	310	CHL	CAC-C3C-C4C	3.06	128.78	124.81
24	g	309	CHL	C1D-CHD-C4C	-3.06	119.47	126.06
31	c	614	8CT	C05-C04-C03	3.06	115.18	110.48
26	7	303	0IE	C9-C10-C11	3.05	129.73	123.47
24	2	309	CHL	CMB-C2B-C1B	3.05	130.02	125.37
24	3	317	CHL	CHD-C1D-ND	-3.05	121.65	124.45
24	8	303	CHL	CHD-C1D-ND	-3.05	121.65	124.45
24	6	317	CHL	OBD-CAD-C3D	-3.05	121.17	128.52
24	r	307	CHL	CAC-C3C-C4C	3.05	128.77	124.81
24	6	304	CHL	C3B-C4B-NB	3.05	113.35	110.52
24	G	305	CHL	C1D-CHD-C4C	-3.05	119.47	126.06
24	6	309	CHL	CHD-C1D-ND	-3.05	121.65	124.45
24	G	309	CHL	C1D-CHD-C4C	-3.05	119.47	126.06
24	G	312	CHL	CMB-C2B-C1B	3.05	130.02	125.37
24	s	402	CHL	C3B-C4B-NB	3.05	113.35	110.52
24	S	608	CHL	CHD-C4C-NC	3.05	129.01	124.20
24	5	318	CHL	CAC-C3C-C4C	3.05	128.77	124.81
26	R	614	0IE	C22-C12-C11	-3.05	118.65	122.92
29	q	301	0UR	C14-C15-C16	-3.05	122.96	127.31
29	4	301	0UR	O44-C45-C46	3.05	119.66	111.55
31	C	614	8CT	C25-C24-C23	-3.05	113.70	123.22
24	8	307	CHL	CAC-C3C-C4C	3.05	128.77	124.81
24	p	318	CHL	C3B-C4B-NB	3.05	113.34	110.52
24	6	304	CHL	C1D-CHD-C4C	-3.05	119.48	126.06
24	G	311	CHL	C3B-C4B-NB	3.05	113.34	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	301	0UR	C48-C47-C46	-3.05	119.31	125.85
29	n	301	0UR	C48-C47-C46	-3.05	119.31	125.85
24	Y	308	CHL	CMB-C2B-C1B	3.05	130.01	125.37
24	7	306	CHL	CAC-C3C-C4C	3.05	128.76	124.81
24	3	317	CHL	C1D-CHD-C4C	-3.05	119.49	126.06
26	r	315	0IE	C22-C12-C11	-3.05	118.66	122.92
24	p	313	CHL	CHD-C1D-ND	-3.04	121.66	124.45
24	y	309	CHL	CMB-C2B-C1B	3.04	130.01	125.37
29	4	301	0UR	C36-C28-C19	3.04	114.16	109.55
24	s	407	CHL	C3B-C4B-NB	3.04	113.34	110.52
24	Y	308	CHL	C1D-CHD-C4C	-3.04	119.49	126.06
24	N	311	CHL	CAC-C3C-C4C	3.04	128.76	124.81
24	g	305	CHL	C1D-CHD-C4C	-3.04	119.49	126.06
24	p	318	CHL	CHD-C4C-NC	3.04	129.00	124.20
24	p	305	CHL	C1-C2-C3	-3.04	120.78	126.04
24	u	309	CHL	CAC-C3C-C4C	3.04	128.76	124.81
25	b	612	CLA	C3B-C4B-NB	-3.04	107.69	110.52
29	G	301	0UR	C14-C15-C16	-3.04	122.97	127.31
25	b	614	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
24	3	310	CHL	C1D-CHD-C4C	-3.04	119.50	126.06
25	4	314	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	b	615	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
24	S	613	CHL	CAA-C2A-C3A	-3.04	109.00	116.10
26	9	302	0IE	C22-C12-C11	-3.04	118.67	122.92
24	R	605	CHL	C1D-CHD-C4C	-3.04	119.50	126.06
33	i	101	LMG	C8-O7-C10	-3.04	110.31	117.79
24	2	311	CHL	CHD-C1D-ND	-3.04	121.66	124.45
24	r	308	CHL	C1D-CHD-C4C	-3.04	119.50	126.06
29	N	301	0UR	C48-C47-C46	-3.04	119.33	125.85
24	6	310	CHL	C1D-CHD-C4C	-3.04	119.51	126.06
24	8	307	CHL	CHD-C4C-NC	3.04	128.99	124.20
24	1	308	CHL	OBD-CAD-C3D	-3.04	121.21	128.52
24	6	317	CHL	CHD-C1D-ND	-3.03	121.67	124.45
29	7	301	0UR	C48-C47-C46	-3.03	119.34	125.85
24	S	606	CHL	C3B-C4B-NB	3.03	113.33	110.52
24	p	305	CHL	C1D-CHD-C4C	-3.03	119.51	126.06
31	c	614	8CT	C25-C24-C23	-3.03	113.75	123.22
25	1	314	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
31	C	615	8CT	C11-C10-C03	-3.03	118.68	127.20
24	6	309	CHL	OBD-CAD-C3D	-3.03	121.22	128.52
24	g	309	CHL	CAC-C3C-C4C	3.03	128.75	124.81
24	5	306	CHL	OBD-CAD-C3D	-3.03	121.22	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	310	CHL	C3B-C4B-NB	3.03	113.33	110.52
24	7	305	CHL	C1-C2-C3	-3.03	120.80	126.04
24	2	310	CHL	C3B-C4B-NB	3.03	113.33	110.52
24	4	311	CHL	C1D-CHD-C4C	-3.03	119.52	126.06
26	4	302	0IE	C22-C12-C11	-3.03	118.68	122.92
24	N	310	CHL	C1D-CHD-C4C	-3.03	119.52	126.06
24	y	311	CHL	CMB-C2B-C1B	3.03	129.98	125.37
24	3	309	CHL	OBD-CAD-C3D	-3.03	121.23	128.52
24	6	309	CHL	CMB-C2B-C1B	3.03	129.98	125.37
24	9	305	CHL	C3B-C4B-NB	3.03	113.32	110.52
24	u	305	CHL	CMB-C2B-C1B	3.03	129.98	125.37
24	R	602	CHL	CMB-C2B-C1B	3.03	129.98	125.37
24	g	306	CHL	C4-C3-C5	3.03	120.36	115.27
24	q	303	CHL	CHD-C1D-ND	-3.03	121.67	124.45
31	A	608	8CT	C11-C10-C03	-3.03	118.71	127.20
25	y	317	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
26	6	302	0IE	C22-C12-C11	-3.02	118.69	122.92
24	S	601	CHL	OMC-CMC-C2C	-3.02	118.85	125.69
24	u	311	CHL	CAC-C3C-C4C	3.02	128.73	124.81
24	u	309	CHL	C1D-CHD-C4C	-3.02	119.53	126.06
24	9	304	CHL	CHD-C4C-NC	3.02	128.97	124.20
24	g	311	CHL	C1-C2-C3	-3.02	120.81	126.04
24	n	311	CHL	CAC-C3C-C4C	3.02	128.73	124.81
24	p	310	CHL	CHD-C4C-NC	3.02	128.97	124.20
24	N	309	CHL	CMB-C2B-C1B	3.02	129.97	125.37
24	1	311	CHL	C1D-CHD-C4C	-3.02	119.54	126.06
24	p	313	CHL	CHD-C4C-NC	3.02	128.96	124.20
24	5	306	CHL	CHB-C1B-NB	-3.02	121.06	124.26
26	3	303	0IE	C9-C10-C11	3.02	129.66	123.47
25	B	614	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
24	G	311	CHL	OBD-CAD-C3D	-3.02	121.25	128.52
26	u	302	0IE	C20-C3-C4	-3.02	120.94	124.83
24	N	311	CHL	C1D-CHD-C4C	-3.02	119.54	126.06
25	B	615	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
24	7	305	CHL	C1D-CHD-C4C	-3.02	119.54	126.06
26	p	302	0IE	C9-C10-C11	3.02	129.66	123.47
24	N	304	CHL	C4A-NA-C1A	3.02	108.06	106.71
24	g	312	CHL	CMB-C2B-C1B	3.02	129.97	125.37
24	4	310	CHL	C3B-C4B-NB	3.02	113.31	110.52
24	4	317	CHL	C1D-CHD-C4C	-3.02	119.55	126.06
24	n	309	CHL	CHB-C4A-NA	3.02	128.69	124.51
31	c	614	8CT	C30-C31-C32	-3.02	117.75	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	p	301	0UR	C9-C8-C7	-3.02	123.00	127.31
24	1	312	CHL	C4A-NA-C1A	3.02	108.06	106.71
25	Y	316	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
26	7	302	0IE	C9-C10-C11	3.02	129.65	123.47
24	7	313	CHL	CHD-C1D-ND	-3.02	121.68	124.45
24	y	309	CHL	C1D-CHD-C4C	-3.02	119.55	126.06
24	4	317	CHL	OBD-CAD-C3D	-3.02	121.26	128.52
24	3	304	CHL	CHD-C4C-NC	3.01	128.95	124.20
25	b	613	CLA	C3B-C4B-NB	-3.01	107.72	110.52
24	n	311	CHL	C1D-CHD-C4C	-3.01	119.56	126.06
24	3	309	CHL	CMB-C2B-C1B	3.01	129.96	125.37
31	c	615	8CT	C11-C10-C03	-3.01	118.74	127.20
24	2	310	CHL	C1D-CHD-C4C	-3.01	119.56	126.06
24	r	303	CHL	CMB-C2B-C1B	3.01	129.96	125.37
24	u	310	CHL	CHD-C1D-ND	-3.01	121.69	124.45
26	u	302	0IE	C21-C7-C8	-3.01	118.70	122.92
29	2	301	0UR	C36-C28-C19	3.01	114.11	109.55
24	g	310	CHL	OBD-CAD-C3D	-3.01	121.27	128.52
24	S	602	CHL	C1-C2-C3	-3.01	120.83	126.04
24	g	312	CHL	CHD-C4C-NC	3.01	128.95	124.20
24	s	409	CHL	CHD-C4C-NC	3.01	128.95	124.20
25	C	612	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	5	318	CHL	CAA-C2A-C3A	-3.01	109.08	116.10
29	5	301	0UR	C43-C3-C4	-3.01	121.38	125.02
24	r	306	CHL	OBD-CAD-C3D	-3.01	121.28	128.52
24	q	311	CHL	CHD-C4C-NC	3.01	128.94	124.20
24	r	306	CHL	C1D-CHD-C4C	-3.01	119.57	126.06
26	u	302	0IE	C22-C12-C11	-3.01	118.71	122.92
35	a	606	PHO	CMB-C2B-C3B	3.01	130.31	124.68
24	Y	319	CHL	O2A-CGA-CBA	3.01	121.34	111.91
26	n	302	0IE	C22-C12-C11	-3.01	118.71	122.92
24	p	310	CHL	CHD-C1D-ND	-3.01	121.69	124.45
24	7	310	CHL	CHD-C1D-ND	-3.01	121.69	124.45
24	4	309	CHL	C1D-CHD-C4C	-3.01	119.57	126.06
26	N	302	0IE	C20-C3-C4	-3.00	120.96	124.83
24	1	317	CHL	C1D-CHD-C4C	-3.00	119.58	126.06
24	u	305	CHL	CHD-C1D-ND	-3.00	121.69	124.45
25	4	315	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
24	u	305	CHL	C3B-C4B-NB	3.00	113.30	110.52
33	W	201	LMG	C8-O7-C10	-3.00	110.39	117.79
24	4	308	CHL	OBD-CAD-C3D	-3.00	121.29	128.52
24	S	607	CHL	C1D-CHD-C4C	-3.00	119.58	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	301	0UR	C28-C19-C18	-3.00	108.90	112.70
31	x	601	8CT	C19-C20-C21	-3.00	123.03	127.31
24	N	308	CHL	CHD-C4C-NC	3.00	128.93	124.20
25	R	613	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
26	N	302	0IE	C22-C12-C11	-3.00	118.72	122.92
24	1	317	CHL	OBD-CAD-C3D	-3.00	121.30	128.52
26	1	302	0IE	C22-C12-C11	-3.00	118.72	122.92
24	3	304	CHL	C1D-CHD-C4C	-3.00	119.59	126.06
24	8	303	CHL	C1D-CHD-C4C	-3.00	119.59	126.06
24	G	306	CHL	C4-C3-C5	3.00	120.32	115.27
24	8	310	CHL	CHD-C4C-NC	3.00	128.93	124.20
31	S	614	8CT	C01-C02-C07	3.00	119.38	113.62
24	S	601	CHL	CMB-C2B-C1B	3.00	129.94	125.37
24	3	310	CHL	OBD-CAD-C3D	-3.00	121.30	128.52
24	g	309	CHL	CHC-C1C-NC	3.00	128.75	124.20
24	R	605	CHL	OBD-CAD-C3D	-3.00	121.31	128.52
33	d	411	LMG	O7-C10-C11	3.00	117.96	111.50
24	r	302	CHL	C2A-C1A-CHA	-3.00	118.62	123.86
33	w	201	LMG	O8-C28-C29	3.00	121.31	111.91
24	4	304	CHL	CAC-C3C-C4C	3.00	128.70	124.81
24	y	311	CHL	CHB-C4A-NA	2.99	128.65	124.51
25	B	615	CLA	C3B-C4B-NB	-2.99	107.74	110.52
24	R	607	CHL	C1D-CHD-C4C	-2.99	119.60	126.06
24	S	605	CHL	OBD-CAD-C3D	-2.99	121.31	128.52
25	B	612	CLA	C3B-C4B-NB	-2.99	107.74	110.52
29	5	301	0UR	C36-C28-C19	2.99	114.08	109.55
24	r	307	CHL	OBD-CAD-C3D	-2.99	121.32	128.52
24	7	313	CHL	CHD-C4C-NC	2.99	128.92	124.20
24	y	306	CHL	C4-C3-C5	2.99	120.31	115.27
24	N	312	CHL	CHD-C1D-ND	-2.99	121.70	124.45
25	r	314	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
35	A	606	PHO	CMB-C2B-C3B	2.99	130.28	124.68
24	r	303	CHL	OBD-CAD-C3D	-2.99	121.32	128.52
31	X	601	8CT	C07-C02-C03	-2.99	118.39	122.73
32	B	618	SQD	O6-C1-C2	2.99	112.97	108.30
24	n	304	CHL	C2A-C1A-CHA	-2.99	118.63	123.86
24	2	318	CHL	CAA-C2A-C3A	-2.99	109.12	116.10
24	2	311	CHL	C4A-NA-C1A	2.99	108.05	106.71
24	1	309	CHL	C1D-CHD-C4C	-2.99	119.61	126.06
24	N	312	CHL	OBD-CAD-C3D	-2.99	121.33	128.52
24	G	311	CHL	CHD-C4C-NC	2.99	128.91	124.20
24	q	309	CHL	O2A-CGA-CBA	2.99	121.29	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	318	CHL	CHD-C1D-ND	-2.99	121.71	124.45
25	8	314	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	4	317	CHL	CAA-C2A-C3A	-2.99	109.13	116.10
29	6	301	0UR	C24-C25-C26	-2.99	106.21	110.30
29	n	301	0UR	C43-C3-C4	-2.99	121.41	125.02
24	u	306	CHL	CMB-C2B-C1B	2.99	129.92	125.37
24	Y	310	CHL	CHB-C4A-NA	2.99	128.64	124.51
24	G	309	CHL	CAC-C3C-C4C	2.99	128.69	124.81
24	s	414	CHL	CAA-C2A-C3A	-2.99	109.13	116.10
29	1	301	0UR	C36-C28-C19	2.99	114.07	109.55
32	b	618	SQD	O6-C1-C2	2.99	112.97	108.30
25	C	611	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
24	u	312	CHL	C3B-C4B-NB	2.98	113.28	110.52
24	n	312	CHL	CHD-C4C-NC	2.98	128.91	124.20
24	5	310	CHL	C1D-CHD-C4C	-2.98	119.62	126.06
24	9	311	CHL	C3B-C4B-NB	2.98	113.28	110.52
25	B	613	CLA	C3B-C4B-NB	-2.98	107.75	110.52
24	4	312	CHL	C4A-NA-C1A	2.98	108.05	106.71
24	q	303	CHL	CMB-C2B-C1B	2.98	129.91	125.37
24	G	312	CHL	CHD-C4C-NC	2.98	128.90	124.20
26	Y	303	0IE	C22-C12-C11	-2.98	118.75	122.92
25	9	314	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	s	416	8CT	C39-C16-C15	2.98	122.77	118.08
25	B	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	G	310	CHL	OBD-CAD-C3D	-2.98	121.35	128.52
24	1	317	CHL	CAA-C2A-C3A	-2.98	109.14	116.10
26	y	303	0IE	C22-C12-C11	-2.98	118.75	122.92
24	9	309	CHL	CHD-C4C-NC	2.98	128.90	124.20
24	8	303	CHL	CMB-C2B-C1B	2.98	129.91	125.37
24	6	310	CHL	OBD-CAD-C3D	-2.98	121.35	128.52
25	c	607	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
24	4	312	CHL	CHD-C1D-ND	-2.98	121.72	124.45
24	s	406	CHL	OBD-CAD-C3D	-2.98	121.36	128.52
25	3	307	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
24	q	307	CHL	CHD-C4C-NC	2.98	128.89	124.20
31	D	410	8CT	C01-C02-C07	2.98	119.33	113.62
26	q	302	0IE	C22-C12-C11	-2.98	118.75	122.92
24	g	309	CHL	OBD-CAD-C3D	-2.98	121.36	128.52
24	N	312	CHL	CHD-C4C-NC	2.97	128.89	124.20
24	5	311	CHL	C4A-NA-C1A	2.97	108.04	106.71
29	g	301	0UR	C14-C15-C16	-2.97	123.07	127.31
24	g	313	CHL	C1-C2-C3	-2.97	120.90	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	305	CHL	OBD-CAD-C3D	-2.97	121.37	128.52
29	8	301	0UR	C14-C15-C16	-2.97	123.07	127.31
29	1	301	0UR	O44-C45-C46	2.97	119.45	111.55
24	7	311	CHL	C3B-C4B-NB	2.97	113.27	110.52
24	q	303	CHL	C1D-CHD-C4C	-2.97	119.65	126.06
24	2	318	CHL	OBD-CAD-C3D	-2.97	121.37	128.52
29	Y	301	0UR	C29-C30-C31	-2.97	108.36	111.74
24	n	304	CHL	C1D-CHD-C4C	-2.97	119.65	126.06
24	G	310	CHL	CMB-C2B-C1B	2.97	129.89	125.37
24	7	312	CHL	CMB-C2B-C1B	2.97	129.89	125.37
24	7	311	CHL	CHD-C1D-ND	-2.97	121.73	124.45
24	2	311	CHL	CHD-C4C-NC	2.97	128.88	124.20
26	5	302	0IE	C9-C10-C11	2.97	129.55	123.47
24	5	311	CHL	CHD-C1D-ND	-2.97	121.73	124.45
24	R	602	CHL	OBD-CAD-C3D	-2.97	121.38	128.52
25	C	607	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	4	308	CHL	CAC-C3C-C4C	2.97	128.66	124.81
29	G	301	0UR	C48-C47-C46	-2.97	119.49	125.85
24	u	310	CHL	OBD-CAD-C3D	-2.96	121.39	128.52
24	Y	308	CHL	CHD-C4C-NC	2.96	128.88	124.20
24	g	311	CHL	OBD-CAD-C3D	-2.96	121.39	128.52
24	g	318	CHL	CAA-C2A-C3A	-2.96	109.18	116.10
24	3	308	CHL	CHD-C1D-ND	-2.96	121.73	124.45
25	r	304	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
29	g	301	0UR	C48-C47-C46	-2.96	119.49	125.85
24	n	309	CHL	CMB-C2B-C1B	2.96	129.88	125.37
24	6	309	CHL	C3B-C4B-NB	2.96	113.26	110.52
24	q	308	CHL	C3B-C4B-NB	2.96	113.26	110.52
24	5	312	CHL	C1D-CHD-C4C	-2.96	119.67	126.06
24	S	606	CHL	CMB-C2B-C1B	2.96	129.88	125.37
29	7	301	0UR	C9-C8-C7	-2.96	123.08	127.31
24	6	317	CHL	CHD-C4C-NC	2.96	128.87	124.20
24	2	305	CHL	OBD-CAD-C3D	-2.96	121.39	128.52
29	7	301	0UR	C5-C4-C3	-2.96	123.45	127.00
25	S	616	CLA	C3B-C4B-NB	-2.96	107.77	110.52
25	c	605	CLA	C3B-C4B-NB	-2.96	107.77	110.52
24	5	318	CHL	OBD-CAD-C3D	-2.96	121.40	128.52
24	1	317	CHL	CAC-C3C-C4C	2.96	128.65	124.81
24	5	309	CHL	CHD-C1D-ND	-2.96	121.73	124.45
24	R	605	CHL	CMB-C2B-C1B	2.96	129.88	125.37
24	y	309	CHL	CHD-C4C-NC	2.96	128.87	124.20
24	8	304	CHL	C1-C2-C3	-2.96	120.93	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	312	CHL	OBD-CAD-C3D	-2.96	121.40	128.52
25	5	314	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
24	6	308	CHL	C1D-CHD-C4C	-2.96	119.68	126.06
24	4	304	CHL	CAA-C2A-C3A	-2.96	109.20	116.10
24	9	309	CHL	OBD-CAD-C3D	-2.96	121.41	128.52
24	G	313	CHL	C1-C2-C3	-2.96	120.93	126.04
24	s	406	CHL	CMB-C2B-C1B	2.96	129.87	125.37
31	S	615	8CT	C39-C16-C15	2.96	122.73	118.08
25	q	312	CLA	C3B-C4B-NB	-2.95	107.77	110.52
24	G	311	CHL	C1-C2-C3	-2.95	120.93	126.04
24	1	304	CHL	CAA-C2A-C3A	-2.95	109.20	116.10
31	C	614	8CT	C30-C31-C32	-2.95	117.83	121.47
31	V	401	8CT	C35-C30-C29	-2.95	108.97	112.70
24	R	601	CHL	C2A-C1A-CHA	-2.95	118.69	123.86
29	y	301	0UR	C29-C30-C31	-2.95	108.38	111.74
24	8	315	CHL	OBD-CAD-C3D	-2.95	121.41	128.52
29	2	301	0UR	C43-C3-C4	-2.95	121.45	125.02
24	G	311	CHL	CMB-C2B-C1B	2.95	129.87	125.37
24	3	317	CHL	CHD-C4C-NC	2.95	128.85	124.20
31	X	601	8CT	C19-C20-C21	-2.95	123.10	127.31
25	N	313	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
31	c	614	8CT	C18-C19-C20	-2.95	117.43	123.47
24	u	305	CHL	C2A-C1A-CHA	-2.95	118.70	123.86
24	5	318	CHL	CHD-C1D-ND	-2.95	121.74	124.45
33	d	411	LMG	C7-O1-C1	-2.95	107.98	113.74
24	g	311	CHL	C3B-C4B-NB	2.95	113.25	110.52
25	1	315	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
31	C	613	8CT	C01-C02-C07	2.95	119.28	113.62
29	5	301	0UR	C5-C4-C3	-2.95	123.46	127.00
24	Y	305	CHL	CMB-C2B-C1B	2.95	129.86	125.37
24	s	407	CHL	CMB-C2B-C1B	2.95	129.86	125.37
24	5	311	CHL	CHD-C4C-NC	2.95	128.85	124.20
24	g	311	CHL	CMB-C2B-C1B	2.95	129.86	125.37
24	7	318	CHL	C3B-C4B-NB	2.95	113.25	110.52
24	N	304	CHL	C1D-CHD-C4C	-2.94	119.70	126.06
24	G	318	CHL	CAA-C2A-C3A	-2.94	109.23	116.10
24	3	308	CHL	C1D-CHD-C4C	-2.94	119.71	126.06
29	q	301	0UR	C28-C19-C18	-2.94	108.98	112.70
31	c	613	8CT	C05-C04-C03	2.94	115.01	110.48
33	C	618	LMG	O8-C28-C29	2.94	121.14	111.91
24	6	309	CHL	C4A-NA-C1A	2.94	108.03	106.71
24	G	312	CHL	CHD-C1D-ND	-2.94	121.75	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	309	CHL	CHC-C1C-NC	2.94	128.67	124.20
25	u	315	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	8	308	CHL	C3B-C4B-NB	2.94	113.24	110.52
24	6	308	CHL	CHD-C1D-ND	-2.94	121.75	124.45
24	8	303	CHL	CHD-C4C-NC	2.94	128.84	124.20
26	7	302	0IE	C22-C12-C11	-2.94	118.80	122.92
25	y	308	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	3	302	0IE	C4-C3-C2	-2.94	117.56	120.08
24	g	318	CHL	OBD-CAD-C3D	-2.94	121.45	128.52
25	c	612	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	n	304	CHL	CHD-C1D-ND	-2.94	121.75	124.45
24	1	312	CHL	OBD-CAD-C3D	-2.94	121.45	128.52
24	y	312	CHL	CAC-C3C-C4C	2.94	128.62	124.81
24	Y	319	CHL	CMB-C2B-C1B	2.94	129.84	125.37
29	n	301	0UR	C28-C19-C18	-2.94	108.99	112.70
25	2	314	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
24	5	305	CHL	CMB-C2B-C1B	2.94	129.84	125.37
24	s	402	CHL	CMB-C2B-C1B	2.94	129.84	125.37
24	2	312	CHL	C1D-CHD-C4C	-2.93	119.73	126.06
24	5	309	CHL	C1D-CHD-C4C	-2.93	119.73	126.06
24	4	317	CHL	CAC-C3C-C4C	2.93	128.62	124.81
26	8	302	0IE	C22-C12-C11	-2.93	118.81	122.92
24	2	305	CHL	CMB-C2B-C1B	2.93	129.84	125.37
24	2	309	CHL	C1D-CHD-C4C	-2.93	119.73	126.06
24	n	310	CHL	OBD-CAD-C3D	-2.93	121.46	128.52
33	i	101	LMG	O8-C28-C29	2.93	121.11	111.91
25	b	615	CLA	C3B-C4B-NB	-2.93	107.80	110.52
26	p	302	0IE	C22-C12-C11	-2.93	118.82	122.92
24	q	307	CHL	CMB-C2B-C1B	2.93	129.83	125.37
25	b	605	CLA	C3B-C4B-NB	-2.93	107.80	110.52
24	3	317	CHL	CMB-C2B-C1B	2.93	129.83	125.37
24	r	302	CHL	CHD-C4C-NC	2.93	128.82	124.20
31	C	614	8CT	C18-C19-C20	-2.93	117.48	123.47
24	N	310	CHL	OBD-CAD-C3D	-2.93	121.48	128.52
25	R	603	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
24	y	318	CHL	CMB-C2B-C1B	2.93	129.82	125.37
24	n	317	CHL	CHC-C4B-NB	-2.93	121.16	124.26
24	6	304	CHL	CHD-C4C-NC	2.93	128.81	124.20
31	C	615	8CT	C10-C11-C12	-2.92	121.82	126.23
24	p	312	CHL	CMB-C2B-C1B	2.92	129.82	125.37
25	s	417	CLA	C3B-C4B-NB	-2.92	107.80	110.52
24	8	307	CHL	C1D-CHD-C4C	-2.92	119.75	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	318	CHL	OBD-CAD-C3D	-2.92	121.48	128.52
29	n	301	0UR	C29-C30-C31	-2.92	108.41	111.74
24	r	302	CHL	CHD-C1D-ND	-2.92	121.77	124.45
24	R	606	CHL	OBD-CAD-C3D	-2.92	121.49	128.52
24	4	304	CHL	OBD-CAD-C3D	-2.92	121.49	128.52
25	Y	315	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	2	309	CHL	CHD-C1D-ND	-2.92	121.77	124.45
24	G	311	CHL	O2A-CGA-CBA	2.92	121.08	111.91
24	6	312	CHL	OBD-CAD-C3D	-2.92	121.49	128.52
24	1	310	CHL	OBD-CAD-C3D	-2.92	121.49	128.52
24	6	304	CHL	OBD-CAD-C3D	-2.92	121.49	128.52
24	q	308	CHL	OBD-CAD-C3D	-2.92	121.49	128.52
24	g	305	CHL	C1-C2-C3	-2.92	120.99	126.04
24	n	308	CHL	CAC-C3C-C4C	2.92	128.60	124.81
24	q	307	CHL	C1D-CHD-C4C	-2.92	119.76	126.06
31	s	415	8CT	C01-C02-C07	2.92	119.22	113.62
24	6	309	CHL	CHD-C4C-NC	2.92	128.80	124.20
25	C	605	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
31	D	410	8CT	C30-C31-C32	-2.92	117.88	121.47
24	S	605	CHL	CMB-C2B-C1B	2.92	129.81	125.37
24	2	313	CHL	CHD-C4C-NC	2.92	128.80	124.20
24	q	303	CHL	CHD-C4C-NC	2.92	128.80	124.20
24	G	309	CHL	OBD-CAD-C3D	-2.92	121.50	128.52
24	1	309	CHL	CHC-C4B-NB	-2.92	121.17	124.26
24	3	308	CHL	OBD-CAD-C3D	-2.92	121.50	128.52
26	2	302	0IE	C9-C10-C11	2.92	129.45	123.47
24	G	305	CHL	C1-C2-C3	-2.92	121.00	126.04
24	Y	311	CHL	CAC-C3C-C4C	2.91	128.59	124.81
24	R	601	CHL	CHD-C4C-NC	2.91	128.79	124.20
31	c	615	8CT	C10-C11-C12	-2.91	121.83	126.23
24	1	312	CHL	C3B-C4B-NB	2.91	113.22	110.52
25	B	605	CLA	C3B-C4B-NB	-2.91	107.81	110.52
24	Y	317	CHL	CMB-C2B-C1B	2.91	129.80	125.37
24	1	312	CHL	CHD-C1D-ND	-2.91	121.78	124.45
24	u	318	CHL	OBD-CAD-C3D	-2.91	121.51	128.52
24	y	309	CHL	OBD-CAD-C3D	-2.91	121.51	128.52
25	n	313	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
37	C	619	DGD	C2G-O2G-C1B	-2.91	110.62	117.79
26	3	302	0IE	C20-C3-C4	-2.91	121.08	124.83
24	4	309	CHL	CHD-C4C-NC	2.91	128.79	124.20
25	a	605	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	N	308	CHL	CMB-C2B-C1B	2.91	129.80	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	613	8CT	C11-C10-C03	-2.91	119.03	127.20
24	9	309	CHL	CHD-C1D-ND	-2.91	121.78	124.45
24	5	313	CHL	CHD-C4C-NC	2.91	128.78	124.20
24	g	306	CHL	CMB-C2B-C1B	2.91	129.80	125.37
25	9	316	CLA	C3B-C4B-NB	-2.91	107.82	110.52
25	C	605	CLA	C3B-C4B-NB	-2.91	107.82	110.52
25	c	605	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
24	8	304	CHL	CHB-C1B-NB	-2.91	121.18	124.26
24	g	310	CHL	CMB-C2B-C1B	2.91	129.79	125.37
24	R	601	CHL	CMB-C2B-C1B	2.90	129.79	125.37
31	c	613	8CT	C11-C10-C03	-2.90	119.05	127.20
24	2	305	CHL	C1D-CHD-C4C	-2.90	119.79	126.06
25	q	305	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
24	y	310	CHL	CHB-C1B-NB	-2.90	121.18	124.26
24	4	310	CHL	CMB-C2B-C1B	2.90	129.79	125.37
25	B	610	CLA	C3B-C4B-NB	-2.90	107.82	110.52
30	d	408	LHG	C5-O7-C7	-2.90	110.65	117.79
24	4	310	CHL	OBD-CAD-C3D	-2.90	121.54	128.52
24	N	308	CHL	C1D-CHD-C4C	-2.90	119.80	126.06
29	8	301	0UR	C28-C19-C18	-2.90	109.03	112.70
24	q	316	CHL	OBD-CAD-C3D	-2.90	121.54	128.52
24	3	309	CHL	C3B-C4B-NB	2.90	113.21	110.52
29	q	301	0UR	C24-C25-C26	-2.90	106.33	110.30
24	q	309	CHL	OBD-CAD-C3D	-2.90	121.54	128.52
24	R	601	CHL	CHD-C1D-ND	-2.90	121.79	124.45
24	y	306	CHL	CMB-C2B-C1B	2.90	129.78	125.37
31	v	401	8CT	C14-C13-C12	-2.90	123.17	127.31
24	8	303	CHL	OBD-CAD-C3D	-2.90	121.54	128.52
25	y	316	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	g	311	CHL	O2A-CGA-CBA	2.90	121.00	111.91
29	3	301	0UR	O44-C45-C46	2.90	119.26	111.55
24	R	607	CHL	CMB-C2B-C1B	2.90	129.78	125.37
24	y	310	CHL	OBD-CAD-C3D	-2.90	121.55	128.52
25	8	311	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	3	305	CHL	CMB-C2B-C1B	2.90	129.78	125.37
24	q	309	CHL	CMB-C2B-C1B	2.90	129.78	125.37
29	5	301	0UR	O44-C45-C46	2.90	119.25	111.55
24	Y	308	CHL	OBD-CAD-C3D	-2.90	121.55	128.52
31	v	401	8CT	C35-C30-C29	-2.90	109.04	112.70
24	3	304	CHL	OBD-CAD-C3D	-2.89	121.55	128.52
25	b	610	CLA	C3B-C4B-NB	-2.89	107.83	110.52
24	u	305	CHL	C1D-CHD-C4C	-2.89	119.81	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	316	CHL	CMB-C2B-C1B	2.89	129.78	125.37
31	a	608	8CT	C25-C24-C23	-2.89	114.19	123.22
24	n	317	CHL	OBD-CAD-C3D	-2.89	121.56	128.52
25	d	405	CLA	C3B-C4B-NB	-2.89	107.83	110.52
33	d	401	LMG	C8-O7-C10	-2.89	110.67	117.79
24	n	308	CHL	CHD-C4C-NC	2.89	128.76	124.20
24	4	317	CHL	CMB-C2B-C1B	2.89	129.77	125.37
24	r	309	CHL	CAC-C3C-C4C	2.89	128.56	124.81
24	9	317	CHL	OBD-CAD-C3D	-2.89	121.56	128.52
25	c	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	N	317	CHL	CHC-C4B-NB	-2.89	121.20	124.26
24	Y	309	CHL	CHB-C4A-NA	2.89	128.51	124.51
35	A	606	PHO	O1D-CGD-CBD	2.89	129.55	124.74
24	N	305	CHL	C1-C2-C3	-2.89	121.04	126.04
24	4	308	CHL	CMB-C2B-C1B	2.89	129.77	125.37
32	A	609	SQD	C44-O6-C1	2.89	119.39	113.74
25	q	315	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	3	302	0IE	C9-C10-C11	2.89	129.39	123.47
31	A	608	8CT	C35-C30-C31	2.89	116.59	111.42
24	2	309	CHL	C2A-C1A-CHA	-2.89	118.81	123.86
26	6	302	0IE	C20-C3-C4	-2.89	121.11	124.83
24	9	304	CHL	C1D-CHD-C4C	-2.89	119.83	126.06
24	6	317	CHL	CMB-C2B-C1B	2.89	129.77	125.37
24	g	311	CHL	CHD-C4C-NC	2.89	128.75	124.20
26	5	303	0IE	C20-C3-C4	-2.89	121.11	124.83
25	b	607	CLA	C3B-C4B-NB	-2.89	107.84	110.52
24	S	606	CHL	OBD-CAD-C3D	-2.89	121.58	128.52
24	N	304	CHL	C3B-C4B-NB	2.88	113.19	110.52
24	6	308	CHL	OBD-CAD-C3D	-2.88	121.58	128.52
25	A	610	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	1	312	CHL	CHD-C4C-NC	2.88	128.75	124.20
29	3	301	0UR	C24-C25-C26	-2.88	106.36	110.30
25	3	313	CLA	C3B-C4B-NB	-2.88	107.84	110.52
24	Y	305	CHL	C4-C3-C5	2.88	120.12	115.27
29	2	301	0UR	O44-C45-C46	2.88	119.22	111.55
26	G	302	0IE	C4-C3-C2	-2.88	117.61	120.08
24	Y	319	CHL	OBD-CAD-C3D	-2.88	121.58	128.52
29	q	301	0UR	O44-C45-C46	2.88	119.22	111.55
29	1	301	0UR	C5-C4-C3	-2.88	123.54	127.00
24	1	308	CHL	CAC-C3C-C4C	2.88	128.55	124.81
24	p	309	CHL	OBD-CAD-C3D	-2.88	121.59	128.52
31	S	614	8CT	C40-C12-C13	-2.88	118.89	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	304	CHL	CHD-C4C-NC	2.88	128.74	124.20
35	d	403	PHO	O1D-CGD-CBD	2.88	129.53	124.74
24	N	305	CHL	C3B-C4B-NB	2.88	113.19	110.52
24	p	309	CHL	CMB-C2B-C1B	2.88	129.75	125.37
24	5	305	CHL	C1D-CHD-C4C	-2.88	119.85	126.06
25	Y	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	Y	309	CHL	C3C-C4C-NC	2.88	113.80	110.57
25	C	610	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	n	304	CHL	CHD-C4C-NC	2.88	128.73	124.20
29	9	301	0UR	O44-C45-C46	2.88	119.20	111.55
25	b	612	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	1	308	CHL	CMB-C2B-C1B	2.87	129.75	125.37
26	4	302	0IE	C6-C7-C8	2.87	123.35	118.94
26	y	303	0IE	C6-C7-C8	2.87	123.35	118.94
25	A	605	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	b	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	9	308	CHL	OBD-CAD-C3D	-2.87	121.60	128.52
24	2	309	CHL	OBD-CAD-C3D	-2.87	121.61	128.52
29	6	301	0UR	O44-C45-C46	2.87	119.19	111.55
31	a	608	8CT	C35-C30-C31	2.87	116.56	111.42
25	N	316	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	5	313	CHL	OBD-CAD-C3D	-2.87	121.61	128.52
25	3	313	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	2	318	CHL	C2A-C1A-CHA	-2.87	118.84	123.85
24	r	308	CHL	CMB-C2B-C1B	2.87	129.74	125.37
26	5	303	0IE	C13-C12-C11	2.87	123.35	118.94
24	4	312	CHL	C3B-C4B-NB	2.87	113.18	110.52
24	G	306	CHL	CMB-C2B-C1B	2.87	129.74	125.37
31	A	608	8CT	C25-C24-C23	-2.87	114.26	123.22
25	4	307	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	1	309	CHL	CHD-C4C-NC	2.87	128.73	124.20
26	g	302	0IE	C4-C3-C2	-2.87	117.61	120.08
24	r	302	CHL	CMB-C2B-C1B	2.87	129.74	125.37
24	p	311	CHL	C4A-NA-C1A	2.87	108.00	106.71
24	9	317	CHL	CHC-C4B-NB	-2.87	121.22	124.26
25	2	317	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	n	309	CHL	OBD-CAD-C3D	-2.87	121.62	128.52
24	S	607	CHL	CMB-C2B-C1B	2.87	129.74	125.37
24	N	317	CHL	OBD-CAD-C3D	-2.87	121.62	128.52
24	7	309	CHL	CMB-C2B-C1B	2.87	129.74	125.37
25	Y	316	CLA	C3B-C4B-NB	-2.87	107.86	110.52
24	N	312	CHL	C1-C2-C3	-2.87	121.09	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	305	CHL	CMB-C2B-C1B	2.87	129.73	125.37
25	a	605	CLA	C3B-C4B-NB	-2.87	107.86	110.52
24	G	309	CHL	CHC-C4B-NB	-2.86	121.22	124.26
31	t	101	8CT	C04-C03-C02	-2.86	118.58	122.61
31	a	608	8CT	C04-C03-C02	-2.86	118.58	122.61
25	a	610	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
24	8	307	CHL	CMB-C2B-C1B	2.86	129.73	125.37
24	2	310	CHL	CAA-C2A-C3A	-2.86	109.42	116.10
24	y	312	CHL	O2A-CGA-CBA	2.86	120.89	111.91
24	N	308	CHL	CAC-C3C-C4C	2.86	128.52	124.81
24	n	310	CHL	CHD-C4C-NC	2.86	128.71	124.20
24	1	310	CHL	CMB-C2B-C1B	2.86	129.73	125.37
24	g	309	CHL	CHC-C4B-NB	-2.86	121.23	124.26
24	p	311	CHL	C3B-C4B-NB	2.86	113.17	110.52
29	1	301	0UR	C48-C47-C46	-2.86	119.72	125.85
24	q	303	CHL	OBD-CAD-C3D	-2.86	121.64	128.52
24	7	318	CHL	CAA-C2A-C3A	-2.86	109.43	116.10
24	2	309	CHL	CHD-C4C-NC	2.86	128.71	124.20
24	3	310	CHL	C3B-C4B-NB	2.86	113.17	110.52
25	n	316	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
35	D	403	PHO	O1D-CGD-CBD	2.86	129.50	124.74
29	9	301	0UR	C48-C47-C46	-2.86	119.72	125.85
24	u	305	CHL	OBD-CAD-C3D	-2.86	121.64	128.52
33	w	201	LMG	C8-O7-C10	-2.86	110.76	117.79
31	X	601	8CT	C01-C02-C07	2.86	119.10	113.62
25	c	603	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	6	305	CHL	C3B-C4B-NB	2.86	113.17	110.52
24	u	310	CHL	CHD-C4C-NC	2.86	128.70	124.20
24	1	304	CHL	OBD-CAD-C3D	-2.86	121.65	128.52
24	5	309	CHL	OBD-CAD-C3D	-2.86	121.65	128.52
26	6	302	0IE	C9-C10-C11	2.86	129.32	123.47
25	5	317	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
24	G	310	CHL	CHD-C4C-NC	2.85	128.70	124.20
24	g	310	CHL	CHD-C4C-NC	2.85	128.70	124.20
25	c	608	CLA	C3B-C4B-NB	-2.85	107.87	110.52
25	C	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
24	3	317	CHL	CAA-C2A-C3A	-2.85	109.44	116.10
24	q	304	CHL	CHB-C1B-NB	-2.85	121.24	124.26
24	R	606	CHL	CMB-C2B-C1B	2.85	129.72	125.37
24	S	602	CHL	C4-C3-C5	2.85	120.07	115.27
24	4	312	CHL	CHD-C4C-NC	2.85	128.70	124.20
24	6	317	CHL	CAA-C2A-C3A	-2.85	109.44	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	309	CHL	CHC-C4B-NB	-2.85	121.24	124.26
24	6	305	CHL	CHD-C1D-ND	-2.85	121.83	124.45
25	g	308	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	5	301	0UR	C24-C25-C26	-2.85	106.40	110.30
26	1	302	0IE	C6-C7-C8	2.85	123.32	118.94
24	u	311	CHL	CMB-C2B-C1B	2.85	129.71	125.37
24	R	608	CHL	CAC-C3C-C4C	2.85	128.51	124.81
24	Y	312	CHL	C1-C2-C3	-2.85	121.11	126.04
25	g	317	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	2	303	0IE	C20-C3-C4	-2.85	121.16	124.83
24	N	304	CHL	CHD-C1D-ND	-2.85	121.83	124.45
24	u	310	CHL	CHC-C4B-NB	-2.85	121.24	124.26
24	N	310	CHL	CHD-C4C-NC	2.85	128.69	124.20
24	u	305	CHL	CHD-C4C-NC	2.85	128.69	124.20
24	2	318	CHL	CHD-C4C-NC	2.85	128.69	124.20
26	G	302	0IE	C6-C7-C8	2.85	123.31	118.94
37	C	620	DGD	O6D-C1D-C2D	-2.85	104.32	110.35
29	8	301	0UR	O44-C45-C46	2.85	119.13	111.55
31	s	415	8CT	C40-C12-C13	-2.85	118.93	122.92
24	q	309	CHL	C6-C5-C3	-2.85	109.96	114.62
24	q	303	CHL	C4A-NA-C1A	2.85	107.99	106.71
24	5	318	CHL	C2A-C1A-CHA	-2.85	118.88	123.85
25	b	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	2	311	CHL	C3B-C4B-NB	2.85	113.16	110.52
24	G	313	CHL	C3B-C4B-NB	2.85	113.16	110.52
25	B	607	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	1	317	CHL	CMB-C2B-C1B	2.85	129.70	125.37
24	r	306	CHL	CMB-C2B-C1B	2.85	129.70	125.37
24	3	309	CHL	CHD-C4C-NC	2.85	128.69	124.20
28	u	304	NEX	C26-C27-C28	2.85	132.01	125.99
29	u	301	0UR	O44-C45-C46	2.85	119.12	111.55
31	A	608	8CT	C04-C03-C02	-2.84	118.61	122.61
24	n	312	CHL	C1-C2-C3	-2.84	121.12	126.04
24	3	312	CHL	OBD-CAD-C3D	-2.84	121.68	128.52
31	d	410	8CT	C30-C31-C32	-2.84	117.97	121.47
25	C	608	CLA	C3B-C4B-NB	-2.84	107.88	110.52
24	u	306	CHL	CHD-C1D-ND	-2.84	121.84	124.45
24	9	310	CHL	CMB-C2B-C1B	2.84	129.70	125.37
28	p	304	NEX	C26-C27-C28	2.84	132.00	125.99
29	N	301	0UR	C29-C30-C31	-2.84	108.51	111.74
24	r	306	CHL	CHD-C1D-ND	-2.84	121.84	124.45
24	g	305	CHL	CMB-C2B-C1B	2.84	129.70	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	314	CLA	C3B-C4B-NB	-2.84	107.88	110.52
24	Y	310	CHL	C4-C3-C5	2.84	120.05	115.27
25	c	606	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	Y	319	CHL	C6-C5-C3	-2.84	109.97	114.62
31	V	401	8CT	C14-C13-C12	-2.84	123.26	127.31
24	s	403	CHL	C4-C3-C5	2.84	120.05	115.27
29	8	301	0UR	C24-C25-C26	-2.84	106.42	110.30
26	p	302	0IE	C6-C7-C8	2.84	123.30	118.94
25	3	316	CLA	C3B-C4B-NB	-2.84	107.88	110.52
25	9	307	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	8	315	CHL	CMB-C2B-C1B	2.84	129.69	125.37
24	6	305	CHL	CMB-C2B-C1B	2.84	129.69	125.37
25	G	307	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	n	307	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	g	302	0IE	C6-C7-C8	2.84	123.30	118.94
24	5	318	CHL	CHD-C4C-NC	2.84	128.67	124.20
25	B	611	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	u	318	CHL	CHC-C4B-NB	-2.84	121.25	124.26
24	n	305	CHL	C1-C2-C3	-2.84	121.14	126.04
24	u	309	CHL	OBD-CAD-C3D	-2.84	121.69	128.52
24	1	308	CHL	CHD-C4C-NC	2.84	128.67	124.20
24	s	408	CHL	CMB-C2B-C1B	2.84	129.69	125.37
29	u	301	0UR	C48-C47-C46	-2.84	119.77	125.85
25	G	317	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
25	C	606	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
24	Y	319	CHL	CHD-C1D-ND	-2.83	121.85	124.45
35	A	606	PHO	O2D-CGD-O1D	-2.83	118.30	123.84
24	q	303	CHL	C1-C2-C3	-2.83	121.14	126.04
24	n	308	CHL	C2A-C1A-CHA	-2.83	118.90	123.86
29	2	301	0UR	C5-C4-C3	-2.83	123.60	127.00
24	Y	311	CHL	O2A-CGA-CBA	2.83	120.80	111.91
25	1	307	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	G	304	NEX	C26-C27-C28	2.83	131.98	125.99
24	u	311	CHL	CHD-C4C-NC	2.83	128.67	124.20
24	8	303	CHL	C1-C2-C3	-2.83	121.14	126.04
28	5	304	NEX	C26-C27-C28	2.83	131.98	125.99
26	Y	303	0IE	C6-C7-C8	2.83	123.29	118.94
24	S	608	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	s	406	CHL	CHD-C1D-ND	-2.83	121.85	124.45
24	n	304	CHL	C3B-C4B-NB	2.83	113.14	110.52
24	6	308	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	u	312	CHL	CMB-C2B-C1B	2.83	129.68	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	312	CHL	C3B-C4B-NB	2.83	113.14	110.52
24	6	310	CHL	C3B-C4B-NB	2.83	113.14	110.52
25	G	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
37	C	620	DGD	O1G-C1A-C2A	2.83	120.79	111.91
24	3	305	CHL	CHD-C1D-ND	-2.83	121.85	124.45
24	s	407	CHL	OBD-CAD-C3D	-2.83	121.71	128.52
24	4	311	CHL	CHD-C1D-ND	-2.83	121.86	124.45
26	5	302	0IE	C6-C7-C8	2.83	123.28	118.94
25	S	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	8	313	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	D	405	CLA	C3B-C4B-NB	-2.83	107.89	110.52
28	R	616	NEX	C26-C27-C28	2.83	131.97	125.99
24	9	311	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	r	307	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	R	601	CHL	OBD-CAD-C3D	-2.83	121.72	128.52
24	7	309	CHL	OBD-CAD-C3D	-2.83	121.72	128.52
25	8	305	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	5	310	CHL	CAA-C2A-C3A	-2.83	109.50	116.10
24	2	311	CHL	OBD-CAD-C3D	-2.83	121.72	128.52
24	S	605	CHL	CHD-C1D-ND	-2.83	121.86	124.45
24	r	302	CHL	OBD-CAD-C3D	-2.83	121.72	128.52
29	2	301	0UR	C24-C25-C26	-2.83	106.44	110.30
24	y	311	CHL	C4-C3-C5	2.83	120.02	115.27
25	N	306	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
24	2	313	CHL	OBD-CAD-C3D	-2.82	121.72	128.52
25	A	605	CLA	C3B-C4B-NB	-2.82	107.89	110.52
26	r	315	0IE	C4-C3-C2	-2.82	117.66	120.08
25	q	314	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
24	s	403	CHL	O2A-CGA-CBA	2.82	120.77	111.91
25	c	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
29	N	301	0UR	C24-C25-C26	-2.82	106.44	110.30
28	2	304	NEX	C26-C27-C28	2.82	131.96	125.99
24	n	310	CHL	O2A-CGA-CBA	2.82	120.76	111.91
24	n	308	CHL	CMB-C2B-C1B	2.82	129.67	125.37
25	b	616	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	8	302	0IE	C10-C9-C8	2.82	129.25	123.47
24	Y	309	CHL	OBD-CAD-C3D	-2.82	121.73	128.52
24	8	310	CHL	C4-C3-C5	2.82	120.02	115.27
24	n	304	CHL	OBD-CAD-C3D	-2.82	121.73	128.52
24	N	308	CHL	OBD-CAD-C3D	-2.82	121.73	128.52
28	r	317	NEX	C26-C27-C28	2.82	131.96	125.99
25	B	611	CLA	C3B-C4B-NB	-2.82	107.90	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	305	CHL	OBD-CAD-C3D	-2.82	121.73	128.52
26	2	303	0IE	C13-C12-C11	2.82	123.27	118.94
24	n	305	CHL	C4-C3-C5	2.82	120.01	115.27
24	q	311	CHL	C4-C3-C5	2.82	120.01	115.27
24	5	309	CHL	CHD-C4C-NC	2.82	128.65	124.20
31	x	601	8CT	C01-C02-C07	2.82	119.03	113.62
28	g	304	NEX	C26-C27-C28	2.82	131.95	125.99
25	1	316	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	7	303	0IE	C20-C3-C4	-2.82	121.20	124.83
25	B	616	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	n	306	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
37	C	619	DGD	O5D-C6D-C5D	2.82	114.26	109.05
25	N	307	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	y	310	CHL	C3C-C4C-NC	2.82	113.73	110.57
25	p	315	CLA	CHB-C4A-NA	2.82	128.41	124.51
24	7	311	CHL	OBD-CAD-C3D	-2.82	121.74	128.52
25	4	316	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	R	601	CHL	C3B-C4B-NB	2.82	113.13	110.52
25	6	316	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	u	315	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	r	312	CLA	C3B-C4B-NB	-2.82	107.90	110.52
24	n	311	CHL	CMB-C2B-C1B	2.82	129.66	125.37
25	7	307	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
28	1	303	NEX	C26-C27-C28	2.82	131.94	125.99
24	n	310	CHL	CMB-C2B-C1B	2.81	129.66	125.37
25	5	314	CLA	C3B-C4B-NB	-2.81	107.90	110.52
24	N	305	CHL	C4-C3-C5	2.81	120.00	115.27
25	9	315	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	u	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	b	606	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	9	319	NEX	C26-C27-C28	2.81	131.94	125.99
25	p	307	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	s	410	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	N	311	CHL	CMB-C2B-C1B	2.81	129.65	125.37
24	5	311	CHL	OBD-CAD-C3D	-2.81	121.75	128.52
25	6	313	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	q	316	CHL	CHD-C4C-NC	2.81	128.63	124.20
31	S	615	8CT	C19-C18-C17	-2.81	117.71	123.47
24	6	312	CHL	C3B-C4B-NB	2.81	113.12	110.52
25	R	611	CLA	C3B-C4B-NB	-2.81	107.91	110.52
24	s	403	CHL	CMB-C2B-C1B	2.81	129.65	125.37
24	5	312	CHL	CMB-C2B-C1B	2.81	129.65	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	608	8CT	C01-C02-C07	2.81	119.02	113.62
24	8	308	CHL	OBD-CAD-C3D	-2.81	121.76	128.52
31	a	608	8CT	C01-C02-C07	2.81	119.02	113.62
24	S	602	CHL	O2A-CGA-CBA	2.81	120.72	111.91
26	3	303	0IE	C13-C12-C11	2.81	123.25	118.94
24	g	313	CHL	C3B-C4B-NB	2.81	113.12	110.52
24	q	316	CHL	C2A-C1A-CHA	-2.81	118.95	123.85
24	N	304	CHL	OBD-CAD-C3D	-2.81	121.76	128.52
24	9	310	CHL	CHD-C4C-NC	2.81	128.63	124.20
26	Y	303	0IE	C20-C3-C4	-2.81	121.22	124.83
24	6	312	CHL	CHD-C4C-NC	2.81	128.63	124.20
28	4	303	NEX	C26-C27-C28	2.81	131.93	125.99
28	y	304	NEX	C26-C27-C28	2.81	131.93	125.99
24	n	310	CHL	C3B-C4B-NB	2.81	113.12	110.52
25	b	611	CLA	C3B-C4B-NB	-2.81	107.91	110.52
30	a	601	LHG	O8-C23-C24	2.81	120.72	111.91
25	u	316	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	g	312	CHL	CHD-C1D-ND	-2.81	121.88	124.45
28	7	304	NEX	C26-C27-C28	2.81	131.93	125.99
24	y	313	CHL	C1-C2-C3	-2.81	121.19	126.04
24	r	302	CHL	C3B-C4B-NB	2.81	113.12	110.52
24	n	317	CHL	CMB-C2B-C1B	2.80	129.64	125.37
24	p	312	CHL	OMC-CMC-C2C	-2.80	119.34	125.69
25	6	315	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
24	4	308	CHL	CHD-C4C-NC	2.80	128.62	124.20
25	B	601	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	7	310	CHL	CMB-C2B-C1B	2.80	129.64	125.37
28	S	617	NEX	C26-C27-C28	2.80	131.92	125.99
24	p	318	CHL	CAA-C2A-C3A	-2.80	109.56	116.10
24	N	305	CHL	CMB-C2B-C1B	2.80	129.64	125.37
25	6	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	u	306	CHL	OBD-CAD-C3D	-2.80	121.78	128.52
26	p	303	0IE	C13-C12-C11	2.80	123.24	118.94
25	8	312	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	S	602	CHL	C3C-C4C-NC	2.80	113.71	110.57
28	N	303	NEX	C39-C29-C30	-2.80	119.00	122.92
26	7	302	0IE	C6-C7-C8	2.80	123.24	118.94
26	R	614	0IE	C4-C3-C2	-2.80	117.67	120.08
24	N	310	CHL	O2A-CGA-CBA	2.80	120.70	111.91
24	8	309	CHL	O2A-CGA-CBA	2.80	120.69	111.91
25	B	606	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	B	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	302	0IE	C10-C9-C8	2.80	129.21	123.47
24	3	308	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	6	317	CHL	C3B-C4B-NB	2.80	113.11	110.52
24	r	306	CHL	C3B-C4B-NB	2.80	113.11	110.52
24	u	309	CHL	CMB-C2B-C1B	2.80	129.63	125.37
35	a	606	PHO	O2D-CGD-O1D	-2.80	118.37	123.84
24	1	304	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	9	308	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	N	317	CHL	CMB-C2B-C1B	2.80	129.63	125.37
28	3	318	NEX	C5-C4-C3	-2.80	108.44	111.75
25	p	314	CLA	C3B-C4B-NB	-2.80	107.92	110.52
28	6	303	NEX	C39-C29-C30	-2.79	119.01	122.92
24	r	309	CHL	CMB-C2B-C1B	2.79	129.62	125.37
33	D	401	LMG	C8-O7-C10	-2.79	110.91	117.79
24	2	318	CHL	CMB-C2B-C1B	2.79	129.62	125.37
24	n	311	CHL	O2A-CGA-CBA	2.79	120.67	111.91
29	p	301	0UR	O44-C45-C46	2.79	118.98	111.55
24	n	304	CHL	C4-C3-C5	2.79	119.97	115.27
24	Y	311	CHL	CMB-C2B-C1B	2.79	129.62	125.37
25	g	316	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	s	413	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	A	609	SQD	O8-S-C6	2.79	110.19	105.74
29	7	301	0UR	O44-C45-C46	2.79	118.98	111.55
24	8	310	CHL	CHD-C1D-ND	-2.79	121.89	124.45
24	N	311	CHL	O2A-CGA-CBA	2.79	120.67	111.91
39	D	406	PL9	C27-C28-C29	-2.79	120.94	127.66
25	C	602	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
29	4	301	0UR	C5-C4-C3	-2.79	123.65	127.00
25	C	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	C	616	CLA	C3B-C4B-NB	-2.79	107.93	110.52
25	7	315	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	S	612	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
28	r	301	NEX	C39-C29-C30	-2.79	119.02	122.92
24	u	311	CHL	C3B-C4B-NB	2.79	113.10	110.52
28	N	303	NEX	C5-C4-C3	-2.79	108.44	111.75
25	7	308	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
37	c	618	DGD	C2G-O2G-C1B	-2.79	110.93	117.79
24	p	311	CHL	OBD-CAD-C3D	-2.79	121.81	128.52
24	3	308	CHL	CHD-C4C-NC	2.79	128.60	124.20
24	4	317	CHL	CHD-C4C-NC	2.79	128.60	124.20
24	3	310	CHL	CMB-C2B-C1B	2.79	129.61	125.37
25	Y	313	CLA	O2D-CGD-O1D	-2.79	118.39	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	305	CHL	C3B-C4B-NB	2.79	113.10	110.52
28	s	401	NEX	C39-C29-C30	-2.79	119.02	122.92
25	3	314	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	b	601	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	s	409	CHL	CMB-C2B-C1B	2.79	129.61	125.37
24	9	309	CHL	CMB-C2B-C1B	2.78	129.61	125.37
26	6	302	0IE	C6-C7-C8	2.78	123.21	118.94
25	B	601	CLA	C3B-C4B-NB	-2.78	107.93	110.52
25	c	603	CLA	C3B-C4B-NB	-2.78	107.93	110.52
25	g	307	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	4	304	CHL	CMB-C2B-C1B	2.78	129.61	125.37
31	s	416	8CT	C19-C18-C17	-2.78	117.78	123.47
24	2	312	CHL	CMB-C2B-C1B	2.78	129.61	125.37
25	q	312	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	6	304	CHL	CHD-C1D-ND	-2.78	121.90	124.45
24	q	310	CHL	O2A-CGA-CBA	2.78	120.64	111.91
25	R	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	S	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	r	311	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	n	303	NEX	C39-C29-C30	-2.78	119.03	122.92
29	1	301	0UR	C43-C3-C4	-2.78	121.66	125.02
35	a	606	PHO	O1D-CGD-CBD	2.78	129.37	124.74
30	y	319	LHG	O8-C23-C24	2.78	120.63	111.91
24	q	311	CHL	OBD-CAD-C3D	-2.78	121.83	128.52
25	p	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	q	313	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	q	303	CHL	C3B-C4B-NB	2.78	113.09	110.52
25	y	317	CLA	C3B-C4B-NB	-2.78	107.94	110.52
39	d	406	PL9	C27-C28-C29	-2.78	120.97	127.66
24	4	304	CHL	CHD-C4C-NC	2.78	128.58	124.20
24	q	307	CHL	C4A-NA-C1A	2.78	107.95	106.71
24	9	309	CHL	CHC-C4B-NB	-2.78	121.32	124.26
24	g	313	CHL	O2A-CGA-CBA	2.78	120.62	111.91
29	y	301	0UR	C48-C47-C46	-2.78	119.89	125.85
31	C	613	8CT	C05-C04-C03	2.78	114.75	110.48
25	S	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
24	3	312	CHL	CMB-C2B-C1B	2.78	129.60	125.37
25	N	315	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	c	602	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	g	317	CLA	C3B-C4B-NB	-2.78	107.94	110.52
28	n	303	NEX	C5-C4-C3	-2.78	108.46	111.75
28	3	318	NEX	C39-C29-C30	-2.78	119.03	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	309	CHL	CMB-C2B-C1B	2.78	129.60	125.37
24	Y	319	CHL	C1-C2-C3	-2.77	121.25	126.04
24	5	318	CHL	CMB-C2B-C1B	2.77	129.59	125.37
26	9	302	0IE	C6-C7-C8	2.77	123.20	118.94
24	q	311	CHL	C1-C2-C3	-2.77	121.25	126.04
29	4	301	0UR	C14-C13-C12	-2.77	118.63	126.42
26	2	302	0IE	C6-C7-C8	2.77	123.19	118.94
31	B	617	8CT	C24-C23-C21	-2.77	118.63	126.42
25	s	404	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	S	613	CHL	CMB-C2B-C1B	2.77	129.59	125.37
24	N	310	CHL	CMB-C2B-C1B	2.77	129.59	125.37
24	8	315	CHL	C2A-C1A-CHA	-2.77	119.02	123.85
24	7	312	CHL	CHB-C4A-NA	2.77	128.34	124.51
24	q	309	CHL	C1-C2-C3	-2.77	121.25	126.04
25	b	601	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	G	313	CHL	O2A-CGA-CBA	2.77	120.60	111.91
25	u	317	CLA	C3B-C4B-NB	-2.77	107.95	110.52
25	y	314	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	9	308	CHL	CHC-C4B-NB	-2.77	121.33	124.26
24	2	318	CHL	C3B-C4B-NB	2.77	113.08	110.52
25	2	315	CLA	C3B-C4B-NB	-2.77	107.95	110.52
25	3	315	CLA	C3B-C4B-NB	-2.77	107.95	110.52
25	4	313	CLA	C3B-C4B-NB	-2.77	107.95	110.52
25	q	306	CLA	C1-C2-C3	-2.77	122.27	126.75
24	5	311	CHL	C3B-C4B-NB	2.77	113.08	110.52
24	s	403	CHL	C3C-C4C-NC	2.77	113.67	110.57
25	u	317	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	s	401	NEX	C5-C4-C3	-2.77	108.47	111.75
24	q	303	CHL	O2A-CGA-CBA	2.77	120.59	111.91
24	u	310	CHL	CMB-C2B-C1B	2.77	129.58	125.37
24	9	305	CHL	CHD-C1D-ND	-2.77	121.91	124.45
24	1	317	CHL	CHD-C4C-NC	2.77	128.56	124.20
29	4	301	0UR	C48-C47-C46	-2.77	119.92	125.85
24	R	608	CHL	CMB-C2B-C1B	2.77	129.58	125.37
24	1	309	CHL	CMB-C2B-C1B	2.76	129.58	125.37
24	9	304	CHL	CHD-C1D-ND	-2.76	121.91	124.45
24	G	305	CHL	C4-C3-C5	2.76	119.92	115.27
25	3	315	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	9	313	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	1	311	CHL	CHD-C1D-ND	-2.76	121.92	124.45
24	1	304	CHL	CHD-C4C-NC	2.76	128.56	124.20
27	r	316	XAT	C31-C30-C29	-2.76	123.37	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	306	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	g	314	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	8	310	CHL	OBD-CAD-C3D	-2.76	121.87	128.52
25	5	315	CLA	C3B-C4B-NB	-2.76	107.95	110.52
24	S	602	CHL	CMB-C2B-C1B	2.76	129.57	125.37
24	N	312	CHL	CMB-C2B-C1B	2.76	129.57	125.37
24	6	310	CHL	CMB-C2B-C1B	2.76	129.57	125.37
25	2	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	S	612	CLA	C3B-C4B-NB	-2.76	107.95	110.52
24	9	304	CHL	OBD-CAD-C3D	-2.76	121.88	128.52
24	8	310	CHL	C1-C2-C3	-2.76	121.27	126.04
31	S	615	8CT	C19-C20-C21	-2.76	123.37	127.31
30	Y	318	LHG	O8-C23-C24	2.76	120.57	111.91
25	n	313	CLA	C3B-C4B-NB	-2.76	107.95	110.52
24	r	303	CHL	CHB-C4A-NA	2.76	128.33	124.51
25	R	604	CLA	CAA-C2A-C3A	-2.76	109.66	116.10
33	C	618	LMG	C8-O7-C10	-2.76	111.00	117.79
25	c	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	y	305	CHL	C4-C3-C5	2.76	119.91	115.27
24	3	317	CHL	C3B-C4B-NB	2.76	113.07	110.52
25	6	313	CLA	C3B-C4B-NB	-2.76	107.96	110.52
25	G	315	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	B	604	CLA	C1-C2-C3	-2.76	121.28	126.04
24	Y	305	CHL	OBD-CAD-C3D	-2.75	121.89	128.52
37	C	619	DGD	O1G-C1A-C2A	2.75	120.55	111.91
25	c	616	CLA	C3B-C4B-NB	-2.75	107.96	110.52
24	1	304	CHL	CHC-C4B-NB	-2.75	121.34	124.26
25	p	314	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	7	318	CHL	CMB-C2B-C1B	2.75	129.56	125.37
24	G	311	CHL	C4-C3-C5	2.75	119.90	115.27
31	T	101	8CT	C01-C02-C07	2.75	118.90	113.62
24	p	318	CHL	OBD-CAD-C3D	-2.75	121.90	128.52
24	8	303	CHL	O2A-CGA-CBA	2.75	120.54	111.91
24	n	312	CHL	CMB-C2B-C1B	2.75	129.56	125.37
25	n	314	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	6	315	CLA	C3B-C4B-NB	-2.75	107.96	110.52
24	y	305	CHL	C3C-C4C-NC	2.75	113.65	110.57
26	2	303	0IE	C6-C7-C8	2.75	123.16	118.94
25	s	413	CLA	C3B-C4B-NB	-2.75	107.97	110.52
28	6	303	NEX	C5-C4-C3	-2.75	108.49	111.75
24	4	309	CHL	CMB-C2B-C1B	2.75	129.55	125.37
24	5	318	CHL	C3B-C4B-NB	2.75	113.06	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	304	CHL	C3C-C4C-NC	2.75	113.65	110.57
24	9	317	CHL	CMB-C2B-C1B	2.75	129.55	125.37
24	g	305	CHL	C4-C3-C5	2.75	119.89	115.27
24	g	311	CHL	C4-C3-C5	2.75	119.89	115.27
24	3	312	CHL	CHD-C4C-NC	2.75	128.53	124.20
28	r	301	NEX	C5-C4-C3	-2.75	108.49	111.75
25	N	313	CLA	C3B-C4B-NB	-2.75	107.97	110.52
31	d	410	8CT	C07-C02-C03	-2.75	118.75	122.73
24	G	309	CHL	CMB-C2B-C1B	2.75	129.55	125.37
24	N	304	CHL	C4-C3-C5	2.75	119.89	115.27
24	y	306	CHL	OBD-CAD-C3D	-2.74	121.92	128.52
29	n	301	0UR	C24-C25-C26	-2.74	106.55	110.30
33	W	201	LMG	O8-C28-C29	2.74	120.52	111.91
37	c	618	DGD	O1G-C1A-C2A	2.74	120.52	111.91
25	N	314	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	S	611	CLA	C3B-C4B-NB	-2.74	107.97	110.52
25	9	316	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	n	315	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	a	604	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
24	r	308	CHL	O2A-CGA-CBA	2.74	120.52	111.91
25	1	314	CLA	C3B-C4B-NB	-2.74	107.97	110.52
25	y	315	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	6	308	CHL	CHD-C4C-NC	2.74	128.52	124.20
25	G	316	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	5	307	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	n	301	0UR	O44-C45-C46	2.74	118.84	111.55
25	7	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	b	606	CLA	C3B-C4B-NB	-2.74	107.97	110.52
25	s	412	CLA	C3B-C4B-NB	-2.74	107.97	110.52
29	Y	301	0UR	C48-C47-C46	-2.74	119.97	125.85
25	G	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	u	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	Y	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	b	608	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	5	309	CHL	C2A-C1A-CHA	-2.74	119.07	123.86
31	t	101	8CT	C01-C02-C07	2.74	118.88	113.62
25	9	313	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	y	312	CHL	CMB-C2B-C1B	2.74	129.54	125.37
25	y	307	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	2	310	CHL	OBD-CAD-C3D	-2.74	121.93	128.52
24	8	315	CHL	CHD-C4C-NC	2.74	128.52	124.20
25	3	316	CLA	O2D-CGD-O1D	-2.74	118.49	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	315	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
25	G	317	CLA	C3B-C4B-NB	-2.74	107.98	110.52
24	s	414	CHL	CMB-C2B-C1B	2.74	129.54	125.37
24	R	607	CHL	O2A-CGA-CBA	2.74	120.50	111.91
30	A	601	LHG	O8-C23-C24	2.74	120.49	111.91
24	6	312	CHL	CMB-C2B-C1B	2.74	129.54	125.37
24	p	318	CHL	CMB-C2B-C1B	2.74	129.54	125.37
24	g	313	CHL	CHD-C4C-NC	2.74	128.51	124.20
24	n	305	CHL	CMB-C2B-C1B	2.74	129.53	125.37
24	p	312	CHL	CHB-C4A-NA	2.73	128.29	124.51
26	3	302	0IE	C6-C7-C8	2.73	123.14	118.94
25	8	306	CLA	C1-C2-C3	-2.73	122.33	126.75
27	R	615	XAT	C15-C14-C13	-2.73	123.41	127.31
25	8	311	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
25	G	316	CLA	C3B-C4B-NB	-2.73	107.98	110.52
37	c	618	DGD	O5D-C6D-C5D	2.73	114.11	109.05
26	Y	302	0IE	C4-C3-C2	-2.73	117.73	120.08
25	b	604	CLA	C1-C2-C3	-2.73	121.32	126.04
24	8	303	CHL	C3B-C4B-NB	2.73	113.05	110.52
24	n	305	CHL	C3B-C4B-NB	2.73	113.05	110.52
24	S	606	CHL	CHD-C1D-ND	-2.73	121.94	124.45
24	5	310	CHL	OBD-CAD-C3D	-2.73	121.95	128.52
25	s	412	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
31	C	613	8CT	C40-C12-C13	-2.73	119.10	122.92
24	y	313	CHL	O2A-CGA-CBA	2.73	120.47	111.91
25	C	603	CLA	C3B-C4B-NB	-2.73	107.98	110.52
24	q	311	CHL	CHD-C1D-ND	-2.73	121.95	124.45
25	9	306	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	u	306	CHL	C4-C3-C5	2.73	119.86	115.27
31	D	410	8CT	C07-C02-C03	-2.73	118.77	122.73
24	q	304	CHL	O2A-CGA-CBA	2.73	120.47	111.91
24	p	306	CHL	OMC-CMC-C2C	-2.73	119.52	125.69
31	c	613	8CT	C40-C12-C13	-2.73	119.11	122.92
24	Y	304	CHL	C4-C3-C5	2.72	119.85	115.27
25	A	604	CLA	CHB-C1B-NB	2.72	127.14	124.26
24	R	602	CHL	CHB-C4A-NA	2.72	128.28	124.51
24	7	318	CHL	OBD-CAD-C3D	-2.72	121.97	128.52
24	R	606	CHL	O2A-CGA-CBA	2.72	120.45	111.91
24	5	313	CHL	CMB-C2B-C1B	2.72	129.52	125.37
24	u	318	CHL	CMB-C2B-C1B	2.72	129.51	125.37
25	1	306	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	A	604	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	303	0IE	C6-C7-C8	2.72	123.12	118.94
27	R	615	XAT	C31-C30-C29	-2.72	123.43	127.31
25	Y	315	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	6	316	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
24	1	305	CHL	CMB-C2B-C1B	2.72	129.51	125.37
25	1	313	CLA	C3B-C4B-NB	-2.72	107.99	110.52
29	1	301	0UR	C14-C13-C12	-2.72	118.78	126.42
24	G	310	CHL	C3B-C4B-NB	2.72	113.04	110.52
24	u	313	CHL	C3B-C4B-NB	2.72	113.04	110.52
25	c	612	CLA	C3B-C4B-NB	-2.72	107.99	110.52
25	c	607	CLA	CHB-C4A-NA	2.72	128.27	124.51
24	p	305	CHL	O2A-CGA-CBA	2.72	120.43	111.91
32	b	618	SQD	O8-S-C6	2.72	110.07	105.74
24	N	310	CHL	C3B-C4B-NB	2.72	113.03	110.52
24	3	310	CHL	CHD-C4C-NC	2.71	128.48	124.20
25	9	314	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	5	316	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	Y	312	CHL	CHD-C1D-ND	-2.71	121.96	124.45
24	u	306	CHL	C3B-C4B-NB	2.71	113.03	110.52
25	2	315	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
31	b	617	8CT	C24-C23-C21	-2.71	118.80	126.42
24	y	313	CHL	CHD-C1D-ND	-2.71	121.96	124.45
24	N	304	CHL	CMB-C2B-C1B	2.71	129.49	125.37
25	6	306	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	Y	317	CHL	CAA-C2A-C3A	-2.71	109.78	116.10
24	q	316	CHL	C3B-C4B-NB	2.71	113.03	110.52
24	2	313	CHL	CMB-C2B-C1B	2.71	129.49	125.37
24	n	305	CHL	OBD-CAD-C3D	-2.71	122.01	128.52
29	q	301	0UR	C48-C47-C46	-2.71	120.05	125.85
25	g	315	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
24	8	304	CHL	O2A-CGA-CBA	2.71	120.40	111.91
25	3	306	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
25	C	612	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	2	311	CHL	CMB-C2B-C1B	2.70	129.49	125.37
24	p	310	CHL	CMB-C2B-C1B	2.70	129.49	125.37
31	T	101	8CT	C04-C03-C02	-2.70	118.81	122.61
25	u	307	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
24	n	304	CHL	CMB-C2B-C1B	2.70	129.48	125.37
24	n	308	CHL	OBD-CAD-C3D	-2.70	122.02	128.52
24	p	312	CHL	C3C-C4C-NC	2.70	113.60	110.57
25	C	607	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	4	304	CHL	CHC-C4B-NB	-2.70	121.40	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	u	314	CLA	C3B-C4B-NB	-2.70	108.01	110.52
25	B	610	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	Y	308	CHL	C4A-NA-C1A	2.70	107.92	106.71
24	8	307	CHL	C3B-C4B-NB	2.70	113.02	110.52
24	2	310	CHL	CMB-C2B-C1B	2.70	129.48	125.37
25	Y	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
29	N	301	0UR	O44-C45-C46	2.70	118.73	111.55
26	9	302	0IE	C20-C3-C4	-2.70	121.36	124.83
33	D	411	LMG	O8-C28-C29	2.70	120.37	111.91
24	6	310	CHL	CHD-C4C-NC	2.70	128.45	124.20
24	5	310	CHL	CMB-C2B-C1B	2.70	129.47	125.37
25	4	314	CLA	C3B-C4B-NB	-2.70	108.01	110.52
26	R	614	0IE	C6-C7-C8	2.70	123.08	118.94
25	a	604	CLA	CHB-C1B-NB	2.69	127.11	124.26
26	G	303	0IE	C9-C10-C11	2.69	128.99	123.47
24	8	303	CHL	C4-C3-C5	2.69	119.80	115.27
24	q	307	CHL	CHD-C1D-ND	-2.69	121.98	124.45
24	y	306	CHL	O2A-CGA-CBA	2.69	120.36	111.91
24	9	305	CHL	C4-C3-C5	2.69	119.80	115.27
25	1	313	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	u	309	CHL	CHD-C4C-NC	2.69	128.45	124.20
24	q	304	CHL	C4-C3-C5	2.69	119.80	115.27
29	u	301	0UR	C43-C3-C4	-2.69	121.77	125.02
25	B	606	CLA	C3B-C4B-NB	-2.69	108.02	110.52
25	7	314	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	7	313	CHL	OBD-CAD-C3D	-2.69	122.04	128.52
25	B	608	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	4	317	CHL	CHC-C4B-NB	-2.69	121.41	124.26
24	r	307	CHL	O2A-CGA-CBA	2.69	120.35	111.91
24	7	312	CHL	C3C-C4C-NC	2.69	113.59	110.57
24	g	305	CHL	OBD-CAD-C3D	-2.69	122.04	128.52
25	y	316	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	9	312	CHL	C3B-C4B-NB	2.69	113.01	110.52
24	u	313	CHL	CMB-C2B-C1B	2.69	129.47	125.37
24	7	306	CHL	OMC-CMC-C2C	-2.69	119.61	125.69
25	C	609	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
29	8	301	0UR	C48-C47-C46	-2.69	120.08	125.85
24	7	306	CHL	C3C-C4C-NC	2.69	113.58	110.57
25	r	305	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
24	4	317	CHL	C4B-CHC-C1C	-2.69	119.96	126.34
25	2	316	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	R	605	CHL	CHB-C4A-NA	2.69	128.23	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	313	CLA	CMB-C2B-C1B	-2.69	121.28	125.37
25	b	610	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
24	G	305	CHL	OBD-CAD-C3D	-2.69	122.06	128.52
24	1	317	CHL	CHC-C4B-NB	-2.69	121.41	124.26
25	b	612	CLA	CHB-C1B-NB	2.69	127.10	124.26
24	9	310	CHL	C3B-C4B-NB	2.69	113.01	110.52
25	C	602	CLA	C3B-C4B-NB	-2.69	108.02	110.52
25	c	610	CLA	C3B-C4B-NB	-2.69	108.02	110.52
29	6	301	0UR	C43-C3-C4	-2.68	121.77	125.02
24	y	310	CHL	CMB-C2B-C1B	2.68	129.46	125.37
24	7	318	CHL	CHD-C1D-ND	-2.68	121.99	124.45
24	y	310	CHL	CHB-C4A-NA	2.68	128.22	124.51
31	c	614	8CT	C24-C25-C26	-2.68	123.48	127.31
24	9	308	CHL	CHD-C4C-NC	2.68	128.43	124.20
25	Y	306	CLA	C3B-C4B-NB	-2.68	108.03	110.52
24	1	317	CHL	C4B-CHC-C1C	-2.68	119.97	126.34
24	y	318	CHL	CAA-C2A-C3A	-2.68	109.84	116.10
26	n	302	0IE	C6-C7-C8	2.68	123.06	118.94
24	5	311	CHL	CMB-C2B-C1B	2.68	129.45	125.37
24	7	305	CHL	O2A-CGA-CBA	2.68	120.32	111.91
31	s	416	8CT	C01-C02-C07	2.68	118.77	113.62
25	R	611	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
29	4	301	0UR	C43-C3-C4	-2.68	121.78	125.02
25	u	307	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	7	315	CLA	C3B-C4B-NB	-2.68	108.03	110.52
24	p	313	CHL	OBD-CAD-C3D	-2.68	122.07	128.52
24	Y	312	CHL	O2A-CGA-CBA	2.68	120.31	111.91
25	C	610	CLA	C3B-C4B-NB	-2.68	108.03	110.52
24	4	305	CHL	CMB-C2B-C1B	2.68	129.45	125.37
24	u	309	CHL	CHC-C4B-NB	-2.68	121.42	124.26
30	d	408	LHG	O8-C23-C24	2.68	120.31	111.91
24	9	305	CHL	OMC-CMC-C2C	-2.68	119.64	125.69
25	3	306	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	9	306	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	g	316	CLA	C3B-C4B-NB	-2.68	108.03	110.52
31	v	401	8CT	C01-C02-C07	2.68	118.76	113.62
25	1	315	CLA	C3B-C4B-NB	-2.68	108.03	110.52
24	G	306	CHL	O2A-CGA-CBA	2.67	120.30	111.91
25	2	316	CLA	C3B-C4B-NB	-2.67	108.03	110.52
25	A	603	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
25	a	603	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
25	A	603	CLA	O2D-CGD-O1D	-2.67	118.61	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	304	CHL	C4-C3-C5	2.67	119.77	115.27
24	n	309	CHL	C3C-C4C-NC	2.67	113.57	110.57
25	y	316	CLA	C3B-C4B-NB	-2.67	108.04	110.52
25	p	315	CLA	C3B-C4B-NB	-2.67	108.04	110.52
26	y	303	0IE	C20-C3-C4	-2.67	121.39	124.83
24	N	305	CHL	OBD-CAD-C3D	-2.67	122.09	128.52
25	R	609	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	G	305	CHL	O2A-CGA-CBA	2.67	120.29	111.91
24	u	312	CHL	CHD-C1D-ND	-2.67	122.00	124.45
24	6	309	CHL	C4B-CHC-C1C	-2.67	120.01	126.34
24	1	312	CHL	CMB-C2B-C1B	2.67	129.43	125.37
24	G	318	CHL	O2D-CGD-O1D	-2.67	118.62	123.84
24	g	305	CHL	O2A-CGA-CBA	2.67	120.28	111.91
24	p	306	CHL	C3C-C4C-NC	2.67	113.56	110.57
25	y	307	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	n	308	CHL	C3B-C4B-NB	2.67	112.99	110.52
24	Y	305	CHL	O2A-CGA-CBA	2.67	120.28	111.91
24	G	309	CHL	CHD-C4C-NC	2.67	128.40	124.20
24	g	309	CHL	CHD-C4C-NC	2.67	128.40	124.20
24	N	317	CHL	C4B-CHC-C1C	-2.67	120.02	126.34
24	q	309	CHL	CHD-C1D-ND	-2.66	122.00	124.45
24	Y	309	CHL	CMB-C2B-C1B	2.66	129.43	125.37
24	3	309	CHL	C4B-CHC-C1C	-2.66	120.02	126.34
24	q	303	CHL	C4-C3-C5	2.66	119.75	115.27
24	Y	308	CHL	CHD-C1D-ND	-2.66	122.01	124.45
24	g	313	CHL	CMB-C2B-C1B	2.66	129.42	125.37
25	r	312	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	7	301	0UR	C43-C3-C4	-2.66	121.80	125.02
24	n	317	CHL	C4B-CHC-C1C	-2.66	120.03	126.34
25	a	607	CLA	C3B-C4B-NB	-2.66	108.05	110.52
25	4	313	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
24	q	304	CHL	CHD-C1D-ND	-2.66	122.01	124.45
24	s	403	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
25	1	313	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	C	609	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	8	302	0IE	C23-C16-C17	2.66	122.27	118.08
24	p	311	CHL	CMB-C2B-C1B	2.66	129.42	125.37
24	y	311	CHL	C1-C2-C3	-2.66	121.44	126.04
24	3	304	CHL	CHD-C1D-ND	-2.66	122.01	124.45
25	c	609	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	N	302	0IE	C6-C7-C8	2.66	123.02	118.94
24	N	308	CHL	C4A-NA-C1A	2.66	107.90	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	307	CHL	C3B-C4B-NB	2.66	112.98	110.52
25	C	604	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	6	309	CHL	O2A-CGA-CBA	2.66	120.25	111.91
32	B	618	SQD	O8-S-C6	2.66	109.97	105.74
24	n	317	CHL	CHD-C4C-NC	2.66	128.39	124.20
24	u	313	CHL	CHD-C4C-NC	2.66	128.39	124.20
25	A	603	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	7	306	CHL	CMB-C2B-C1B	2.66	129.41	125.37
31	s	416	8CT	C19-C20-C21	-2.66	123.52	127.31
24	G	306	CHL	OBD-CAD-C3D	-2.66	122.13	128.52
24	9	312	CHL	CMB-C2B-C1B	2.66	129.41	125.37
26	q	302	0IE	C23-C16-C17	2.65	122.26	118.08
24	3	309	CHL	O2A-CGA-CBA	2.65	120.24	111.91
24	g	306	CHL	O2A-CGA-CBA	2.65	120.24	111.91
24	g	312	CHL	O2A-CGA-CBA	2.65	120.23	111.91
24	8	307	CHL	OBD-CAD-C3D	-2.65	122.14	128.52
24	2	305	CHL	CHD-C1D-ND	-2.65	122.02	124.45
24	G	312	CHL	O2A-CGA-CBA	2.65	120.23	111.91
33	d	401	LMG	O8-C28-C29	2.65	120.23	111.91
24	Y	310	CHL	C3C-C4C-NC	2.65	113.54	110.57
24	9	311	CHL	CHD-C1D-ND	-2.65	122.02	124.45
24	u	305	CHL	C4-C3-C5	2.65	119.73	115.27
25	a	603	CLA	C3B-C4B-NB	-2.65	108.06	110.52
24	p	313	CHL	CMB-C2B-C1B	2.65	129.41	125.37
24	p	310	CHL	C4A-NA-C1A	2.65	107.90	106.71
31	C	615	8CT	C01-C02-C07	2.65	118.70	113.62
30	n	318	LHG	O8-C23-C24	2.65	120.22	111.91
24	p	306	CHL	CMB-C2B-C1B	2.65	129.40	125.37
25	G	314	CLA	C3B-C4B-NB	-2.65	108.06	110.52
24	p	305	CHL	C4-C3-C5	2.65	119.73	115.27
24	8	309	CHL	C3C-C4C-NC	2.65	113.54	110.57
24	G	313	CHL	CHD-C4C-NC	2.65	128.38	124.20
31	V	401	8CT	C24-C25-C26	-2.65	123.53	127.31
24	N	310	CHL	C4-C3-C5	2.65	119.72	115.27
24	Y	310	CHL	C1-C2-C3	-2.65	121.47	126.04
24	7	311	CHL	CMB-C2B-C1B	2.65	129.40	125.37
24	g	306	CHL	OBD-CAD-C3D	-2.65	122.15	128.52
30	D	407	LHG	O8-C23-C24	2.65	120.21	111.91
24	R	602	CHL	CHD-C1D-ND	-2.65	122.02	124.45
25	R	609	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	n	315	CLA	C3B-C4B-NB	-2.65	108.06	110.52
24	4	311	CHL	CMB-C2B-C1B	2.65	129.40	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	607	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	N	318	LHG	O8-C23-C24	2.65	120.21	111.91
25	r	313	CLA	CHB-C4A-NA	2.64	128.17	124.51
24	g	318	CHL	O2D-CGD-O1D	-2.64	118.67	123.84
24	8	304	CHL	CHD-C1D-ND	-2.64	122.02	124.45
25	N	315	CLA	C3B-C4B-NB	-2.64	108.06	110.52
33	m	101	LMG	O8-C28-C29	2.64	120.20	111.91
25	c	609	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	g	310	CHL	C3B-C4B-NB	2.64	112.97	110.52
25	b	616	CLA	CHB-C4A-NA	2.64	128.17	124.51
24	8	304	CHL	C4-C3-C5	2.64	119.72	115.27
25	1	316	CLA	C3B-C4B-NB	-2.64	108.06	110.52
25	p	308	CLA	C1-C2-C3	-2.64	122.48	126.75
25	r	310	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
31	x	601	8CT	C04-C03-C02	-2.64	118.89	122.61
24	9	312	CHL	CHD-C4C-NC	2.64	128.36	124.20
25	y	314	CLA	C3B-C4B-NB	-2.64	108.07	110.52
25	7	317	CLA	C3B-C4B-NB	-2.64	108.07	110.52
24	9	304	CHL	O2A-CGA-CBA	2.64	120.19	111.91
24	4	312	CHL	CMB-C2B-C1B	2.64	129.39	125.37
25	B	616	CLA	CHB-C4A-NA	2.64	128.16	124.51
31	X	601	8CT	C05-C04-C03	2.64	114.54	110.48
24	s	414	CHL	OBD-CAD-C3D	-2.64	122.17	128.52
26	r	315	0IE	C20-C3-C4	-2.64	121.44	124.83
33	B	619	LMG	O8-C28-C29	2.64	120.18	111.91
25	9	315	CLA	C3B-C4B-NB	-2.64	108.07	110.52
25	5	307	CLA	C3B-C4B-NB	-2.64	108.07	110.52
26	g	303	0IE	C9-C10-C11	2.64	128.88	123.47
37	C	619	DGD	C1E-O6E-C5E	-2.64	108.51	113.69
24	7	309	CHL	CHC-C4B-NB	-2.64	121.47	124.26
24	7	313	CHL	CMB-C2B-C1B	2.64	129.38	125.37
24	s	407	CHL	CHD-C1D-ND	-2.64	122.03	124.45
24	N	310	CHL	C1-C2-C3	-2.64	121.48	126.04
31	S	615	8CT	C01-C02-C07	2.64	118.68	113.62
28	N	303	NEX	C31-C30-C29	-2.63	123.55	127.31
25	3	307	CLA	C3B-C4B-NB	-2.63	108.07	110.52
25	B	608	CLA	C3B-C4B-NB	-2.63	108.07	110.52
24	R	608	CHL	CHD-C1D-ND	-2.63	122.03	124.45
24	n	310	CHL	C4-C3-C5	2.63	119.70	115.27
25	6	307	CLA	C3B-C4B-NB	-2.63	108.07	110.52
31	C	614	8CT	C06-C07-C02	-2.63	109.38	114.08
25	A	607	CLA	C3B-C4B-NB	-2.63	108.07	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	409	CHL	CHD-C1D-ND	-2.63	122.04	124.45
31	C	615	8CT	C40-C12-C13	-2.63	119.24	122.92
25	R	603	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	r	304	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	6	303	NEX	C31-C30-C29	-2.63	123.56	127.31
24	5	306	CHL	CMB-C2B-C1B	2.63	129.37	125.37
24	q	308	CHL	CMB-C2B-C1B	2.63	129.37	125.37
24	R	607	CHL	C3C-C4C-NC	2.63	113.52	110.57
24	7	305	CHL	C4-C3-C5	2.63	119.69	115.27
25	u	316	CLA	C3B-C4B-NB	-2.63	108.08	110.52
26	7	303	0IE	C13-C12-C11	2.63	122.97	118.94
24	1	308	CHL	C2A-C1A-CHA	-2.63	119.27	123.86
24	6	308	CHL	C3B-C4B-NB	2.63	112.95	110.52
24	4	308	CHL	C2A-C1A-CHA	-2.62	119.27	123.86
28	r	301	NEX	C31-C30-C29	-2.62	123.56	127.31
26	1	302	0IE	C4-C3-C2	-2.62	117.83	120.08
30	A	612	LHG	O8-C23-C24	2.62	120.14	111.91
25	5	316	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	S	602	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
31	d	410	8CT	C11-C10-C03	-2.62	119.84	127.20
24	3	311	CHL	CMB-C2B-C1B	2.62	129.36	125.37
25	q	305	CLA	C3B-C4B-NB	-2.62	108.08	110.52
39	d	406	PL9	C40-C39-C41	2.62	119.68	115.27
25	S	603	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	g	314	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	u	305	CHL	CHC-C4B-NB	-2.62	121.48	124.26
25	u	308	CLA	C1-C2-C3	-2.62	122.51	126.75
26	r	315	0IE	C6-C7-C8	2.62	122.96	118.94
24	3	309	CHL	CAC-C3C-C4C	2.62	128.21	124.81
24	S	613	CHL	OBD-CAD-C3D	-2.62	122.22	128.52
25	A	607	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	s	417	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	S	608	CHL	CHD-C1D-ND	-2.62	122.05	124.45
24	p	318	CHL	CHD-C1D-ND	-2.62	122.05	124.45
31	A	608	8CT	C35-C30-C29	-2.62	109.39	112.70
25	b	605	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	Y	305	CHL	C3C-C4C-NC	2.62	113.50	110.57
24	5	305	CHL	CHD-C1D-ND	-2.62	122.05	124.45
24	6	311	CHL	CMB-C2B-C1B	2.62	129.35	125.37
29	9	301	0UR	C43-C3-C4	-2.62	121.86	125.02
24	7	306	CHL	O2A-CGA-CBA	2.62	120.11	111.91
24	S	613	CHL	O2D-CGD-O1D	-2.62	118.72	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	307	CLA	C3B-C4B-NB	-2.62	108.09	110.52
30	p	319	LHG	O8-C23-C24	2.61	120.11	111.91
24	n	304	CHL	C1-C2-C3	-2.61	121.52	126.04
25	a	603	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	6	305	CHL	OBD-CAD-C3D	-2.61	122.23	128.52
24	s	409	CHL	OBD-CAD-C3D	-2.61	122.23	128.52
25	8	306	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	p	317	CLA	C3B-C4B-NB	-2.61	108.09	110.52
30	9	318	LHG	O8-C23-C24	2.61	120.11	111.91
24	N	317	CHL	CHD-C4C-NC	2.61	128.32	124.20
25	N	306	CLA	C3B-C4B-NB	-2.61	108.09	110.52
24	N	309	CHL	C3C-C4C-NC	2.61	113.50	110.57
28	s	401	NEX	C31-C30-C29	-2.61	123.58	127.31
25	2	308	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	2	319	LHG	O8-C23-C24	2.61	120.10	111.91
24	8	315	CHL	C3B-C4B-NB	2.61	112.94	110.52
25	6	306	CLA	C3B-C4B-NB	-2.61	108.09	110.52
25	n	306	CLA	C3B-C4B-NB	-2.61	108.09	110.52
30	5	319	LHG	O8-C23-C24	2.61	120.09	111.91
25	b	608	CLA	C3B-C4B-NB	-2.61	108.09	110.52
25	7	316	CLA	C3B-C4B-NB	-2.61	108.09	110.52
24	R	605	CHL	C3C-C4C-NC	2.61	113.50	110.57
28	3	318	NEX	C31-C30-C29	-2.61	123.59	127.31
33	d	411	LMG	C8-O7-C10	-2.61	111.37	117.79
25	c	602	CLA	C3B-C4B-NB	-2.61	108.10	110.52
24	4	304	CHL	C4B-CHC-C1C	-2.61	120.15	126.34
24	s	414	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
24	G	312	CHL	C4A-NA-C1A	2.61	107.88	106.71
24	3	305	CHL	C4B-CHC-C1C	-2.61	120.16	126.34
25	B	607	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	S	614	8CT	C10-C11-C12	2.61	130.17	126.23
24	1	311	CHL	CMB-C2B-C1B	2.61	129.34	125.37
25	D	405	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	R	604	CLA	C3B-C4B-NB	-2.60	108.10	110.52
25	C	608	CLA	CHB-C1B-NB	2.60	127.01	124.26
31	D	410	8CT	C11-C10-C03	-2.60	119.89	127.20
31	V	401	8CT	C01-C02-C07	2.60	118.62	113.62
25	R	604	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	9	317	CHL	CHD-C4C-NC	2.60	128.30	124.20
35	A	606	PHO	C1C-C2C-C3C	-2.60	106.45	108.61
24	p	306	CHL	O2A-CGA-CBA	2.60	120.07	111.91
26	6	302	0IE	C23-C16-C17	2.60	122.17	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	307	CHL	OBD-CAD-C3D	-2.60	122.26	128.52
28	n	303	NEX	C31-C30-C29	-2.60	123.60	127.31
31	c	614	8CT	C06-C07-C02	-2.60	109.44	114.08
25	9	314	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	3	308	CHL	C3B-C4B-NB	2.60	112.93	110.52
25	8	305	CLA	C3B-C4B-NB	-2.60	108.10	110.52
24	r	303	CHL	CHD-C1D-ND	-2.60	122.07	124.45
30	g	319	LHG	O8-C23-C24	2.60	120.06	111.91
25	S	616	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	C	614	8CT	C24-C25-C26	-2.60	123.60	127.31
24	6	305	CHL	C4B-CHC-C1C	-2.60	120.18	126.34
24	u	305	CHL	O2A-CGA-CBA	2.60	120.06	111.91
30	D	408	LHG	O8-C23-C24	2.60	120.06	111.91
31	a	608	8CT	C35-C30-C29	-2.60	109.42	112.70
24	u	318	CHL	CHD-C4C-NC	2.60	128.29	124.20
31	V	401	8CT	C30-C31-C32	-2.60	118.27	121.47
24	1	309	CHL	C4A-NA-C1A	2.60	107.87	106.71
25	Y	315	CLA	C3B-C4B-NB	-2.60	108.11	110.52
25	4	316	CLA	C3B-C4B-NB	-2.60	108.11	110.52
30	7	319	LHG	O8-C23-C24	2.60	120.05	111.91
25	n	307	CLA	C1-C2-C3	-2.60	122.55	126.75
24	2	306	CHL	CMB-C2B-C1B	2.59	129.32	125.37
25	5	316	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	6	315	CLA	CHB-C4A-NA	2.59	128.10	124.51
24	4	310	CHL	CHD-C1D-ND	-2.59	122.07	124.45
24	y	309	CHL	CHD-C1D-ND	-2.59	122.07	124.45
25	8	314	CLA	C3B-C4B-NB	-2.59	108.11	110.52
24	8	309	CHL	CHB-C4A-NA	2.59	128.10	124.51
26	Y	302	0IE	C6-C7-C8	2.59	122.92	118.94
31	A	608	8CT	C27-C26-C28	2.59	122.16	118.08
25	p	316	CLA	C3B-C4B-NB	-2.59	108.11	110.52
31	a	608	8CT	C27-C26-C28	2.59	122.16	118.08
24	6	305	CHL	O2A-CGA-CBA	2.59	120.04	111.91
24	5	306	CHL	CHB-C4A-NA	2.59	128.09	124.51
25	4	313	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	q	306	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
26	4	302	0IE	C4-C3-C2	-2.59	117.86	120.08
29	3	301	0UR	C29-C30-C31	-2.59	108.80	111.74
24	p	309	CHL	CHD-C4C-NC	2.59	128.28	124.20
25	B	612	CLA	CHB-C1B-NB	2.59	127.00	124.26
24	y	311	CHL	C3C-C4C-NC	2.59	113.47	110.57
24	3	305	CHL	OBD-CAD-C3D	-2.59	122.29	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	315	CLA	C3B-C4B-NB	-2.59	108.11	110.52
24	6	317	CHL	C4A-NA-C1A	2.59	107.87	106.71
24	7	311	CHL	C4A-NA-C1A	2.59	107.87	106.71
26	g	302	0IE	C13-C12-C11	2.59	122.91	118.94
26	y	302	0IE	C6-C7-C8	2.59	122.91	118.94
31	v	401	8CT	C24-C25-C26	-2.59	123.62	127.31
25	r	312	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	u	308	CLA	C3B-C4B-NB	-2.59	108.12	110.52
30	a	612	LHG	O8-C23-C24	2.59	120.02	111.91
25	5	308	CLA	CHB-C4A-NA	2.59	128.09	124.51
31	s	415	8CT	C10-C11-C12	2.58	130.14	126.23
25	r	305	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
25	q	315	CLA	C3B-C4B-NB	-2.58	108.12	110.52
29	9	301	0UR	C24-C25-C26	-2.58	106.77	110.30
24	1	310	CHL	CHD-C1D-ND	-2.58	122.08	124.45
33	D	401	LMG	O8-C28-C29	2.58	120.02	111.91
25	c	604	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	G	313	CHL	CMB-C2B-C1B	2.58	129.30	125.37
29	G	301	0UR	C4-C3-C2	-2.58	117.86	120.08
31	B	617	8CT	C40-C12-C13	-2.58	119.31	122.92
31	c	615	8CT	C01-C02-C07	2.58	118.57	113.62
24	u	306	CHL	O2A-CGA-CBA	2.58	120.00	111.91
31	C	614	8CT	C11-C10-C03	-2.58	119.96	127.20
24	Y	319	CHL	C4-C3-C5	2.58	119.61	115.27
24	8	310	CHL	O2A-CGA-CBA	2.58	120.00	111.91
35	D	403	PHO	C1-C2-C3	-2.58	121.58	126.04
30	d	407	LHG	O8-C23-C24	2.58	120.00	111.91
25	u	315	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	B	605	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	r	308	CHL	C3C-C4C-NC	2.58	113.46	110.57
24	5	306	CHL	OMC-CMC-C2C	-2.58	119.86	125.69
25	b	611	CLA	CHB-C4A-NA	2.58	128.07	124.51
24	q	308	CHL	C3C-C4C-NC	2.58	113.46	110.57
25	c	603	CLA	CMB-C2B-C1B	-2.58	121.45	125.37
25	s	411	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	5	313	CHL	C4A-NA-C1A	2.58	107.86	106.71
31	C	613	8CT	C18-C19-C20	-2.58	118.20	123.47
25	N	313	CLA	CHB-C4A-NA	2.58	128.07	124.51
25	C	611	CLA	CHB-C4A-NA	2.58	128.07	124.51
26	y	302	0IE	C4-C3-C2	-2.57	117.87	120.08
26	G	302	0IE	C13-C12-C11	2.57	122.89	118.94
25	c	607	CLA	C3B-C4B-NB	-2.57	108.13	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	608	CLA	CHB-C1B-NB	2.57	126.98	124.26
24	p	306	CHL	OBD-CAD-C3D	-2.57	122.33	128.52
24	R	606	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
24	n	310	CHL	C1-C2-C3	-2.57	121.59	126.04
26	r	315	0IE	C13-C12-C11	2.57	122.89	118.94
24	3	311	CHL	CHD-C1D-ND	-2.57	122.09	124.45
24	p	309	CHL	CHC-C4B-NB	-2.57	121.53	124.26
24	1	304	CHL	C4B-CHC-C1C	-2.57	120.24	126.34
24	7	306	CHL	C4-C3-C5	2.57	119.60	115.27
24	y	306	CHL	C3C-C4C-NC	2.57	113.45	110.57
25	b	606	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	b	607	CLA	CHB-C4A-NA	2.57	128.07	124.51
31	v	401	8CT	C30-C31-C32	-2.57	118.30	121.47
24	p	306	CHL	C4-C3-C5	2.57	119.60	115.27
24	6	309	CHL	CAC-C3C-C4C	2.57	128.15	124.81
24	G	309	CHL	C4B-CHC-C1C	-2.57	120.24	126.34
25	2	316	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	B	601	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	7	316	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	C	603	CLA	CMB-C2B-C1B	-2.57	121.46	125.37
35	a	606	PHO	C1C-C2C-C3C	-2.57	106.48	108.61
24	N	312	CHL	O2A-CGA-CBA	2.57	119.96	111.91
25	g	316	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	q	312	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	Y	303	0IE	C9-C10-C11	2.57	128.73	123.47
24	q	309	CHL	C4-C3-C5	2.57	119.59	115.27
24	8	307	CHL	CHD-C1D-ND	-2.57	122.10	124.45
24	N	309	CHL	CHB-C4A-NA	2.57	128.06	124.51
25	S	611	CLA	CHB-C4A-NA	2.57	128.06	124.51
31	c	614	8CT	C11-C10-C03	-2.57	120.00	127.20
24	Y	309	CHL	CHB-C1B-NB	-2.57	121.54	124.26
24	N	304	CHL	C1-C2-C3	-2.57	121.61	126.04
33	C	618	LMG	C1-O6-C5	-2.56	108.65	113.69
26	R	614	0IE	C20-C3-C4	-2.56	121.53	124.83
24	u	309	CHL	C3B-C4B-NB	2.56	112.89	110.52
25	C	608	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	6	304	CHL	O2A-CGA-CBA	2.56	119.95	111.91
24	2	306	CHL	CHB-C4A-NA	2.56	128.06	124.51
26	3	302	0IE	C23-C16-C17	2.56	122.12	118.08
24	n	312	CHL	O2A-CGA-CBA	2.56	119.95	111.91
24	2	309	CHL	C3B-C4B-NB	2.56	112.89	110.52
25	s	404	CLA	C3B-C4B-NB	-2.56	108.14	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	3	318	NEX	C26-C27-C28	-2.56	120.57	125.99
37	C	620	DGD	C2G-O2G-C1B	-2.56	111.48	117.79
35	d	403	PHO	C1-C2-C3	-2.56	121.61	126.04
24	7	310	CHL	C4A-NA-C1A	2.56	107.86	106.71
24	1	309	CHL	C3B-C4B-NB	2.56	112.89	110.52
26	y	302	0IE	C13-C12-C11	2.56	122.87	118.94
29	p	301	0UR	C43-C3-C4	-2.56	121.92	125.02
24	3	317	CHL	CMA-C3A-C2A	-2.56	110.12	116.10
25	r	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	R	601	CHL	CHC-C4B-NB	-2.56	121.55	124.26
25	s	412	CLA	CHB-C4A-NA	2.56	128.05	124.51
28	6	303	NEX	C26-C27-C28	-2.56	120.58	125.99
25	6	306	CLA	CAA-C2A-C3A	-2.56	110.12	116.10
25	g	307	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	2	315	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	y	318	CHL	C3C-C4C-NC	2.56	113.44	110.57
25	1	307	CLA	C3B-C4B-NB	-2.56	108.14	110.52
39	D	406	PL9	C22-C23-C24	-2.56	121.50	127.66
25	2	308	CLA	C1-C2-C3	-2.56	122.61	126.75
25	9	307	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	6	313	CLA	CAA-C2A-C3A	-2.56	110.13	116.10
25	R	612	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	r	302	CHL	CHC-C4B-NB	-2.56	121.55	124.26
25	3	313	CLA	CAA-C2A-C3A	-2.56	110.13	116.10
24	3	304	CHL	O2A-CGA-CBA	2.56	119.93	111.91
25	3	315	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	5	309	CHL	C4B-CHC-C1C	-2.56	120.28	126.34
32	D	409	SQD	O8-S-C6	2.56	109.81	105.74
25	9	307	CLA	C1-C2-C3	-2.55	122.62	126.75
25	5	317	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	d	405	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	9	309	CHL	C3B-C4B-NB	2.55	112.89	110.52
24	7	309	CHL	C4B-CHC-C1C	-2.55	120.28	126.34
25	C	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	S	613	CHL	CHD-C1D-ND	-2.55	122.11	124.45
24	q	311	CHL	O2A-CGA-CBA	2.55	119.92	111.91
25	Y	307	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	r	301	NEX	C26-C27-C28	-2.55	120.59	125.99
25	6	314	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	8	308	CHL	CMB-C2B-C1B	2.55	129.26	125.37
31	C	615	8CT	C27-C26-C25	-2.55	119.35	122.92
24	7	306	CHL	OBD-CAD-C3D	-2.55	122.38	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	306	CHL	CHD-C1D-ND	-2.55	122.11	124.45
24	3	305	CHL	O2A-CGA-CBA	2.55	119.92	111.91
24	4	309	CHL	C3B-C4B-NB	2.55	112.88	110.52
25	n	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	Y	317	CHL	C3C-C4C-NC	2.55	113.43	110.57
24	q	310	CHL	C3C-C4C-NC	2.55	113.43	110.57
24	2	309	CHL	C4B-CHC-C1C	-2.55	120.29	126.34
24	2	306	CHL	OMC-CMC-C2C	-2.55	119.92	125.69
25	p	317	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	1	317	CHL	C3B-C4B-NB	2.55	112.88	110.52
26	Y	302	0IE	C13-C12-C11	2.55	122.85	118.94
25	q	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	R	602	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
24	4	308	CHL	C4B-CHC-C1C	-2.55	120.29	126.34
31	c	613	8CT	C18-C19-C20	-2.55	118.25	123.47
25	B	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	u	318	CHL	C2A-C1A-CHA	-2.55	119.40	123.85
24	8	303	CHL	C4B-CHC-C1C	-2.55	120.29	126.34
24	g	309	CHL	C4B-CHC-C1C	-2.55	120.29	126.34
24	5	306	CHL	C3C-C4C-NC	2.55	113.43	110.57
31	c	615	8CT	C27-C26-C25	-2.55	119.35	122.92
24	4	304	CHL	C3B-C4B-NB	2.55	112.88	110.52
30	G	319	LHG	O8-C23-C24	2.55	119.90	111.91
25	5	315	CLA	CHB-C4A-NA	2.55	128.03	124.51
39	d	406	PL9	C22-C23-C24	-2.55	121.53	127.66
25	S	609	CLA	C3B-C4B-NB	-2.54	108.15	110.52
25	5	317	CLA	C3B-C4B-NB	-2.54	108.15	110.52
25	s	410	CLA	C3B-C4B-NB	-2.54	108.15	110.52
25	G	316	CLA	CHB-C4A-NA	2.54	128.03	124.51
31	v	401	8CT	C25-C24-C23	-2.54	115.28	123.22
24	S	608	CHL	OBD-CAD-C3D	-2.54	122.40	128.52
24	r	303	CHL	O2D-CGD-O1D	-2.54	118.86	123.84
25	G	317	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	s	401	NEX	C26-C27-C28	-2.54	120.62	125.99
24	8	315	CHL	CHC-C4B-NB	-2.54	121.56	124.26
24	5	309	CHL	C3B-C4B-NB	2.54	112.87	110.52
24	u	310	CHL	C3B-C4B-NB	2.54	112.87	110.52
26	R	614	0IE	C13-C12-C11	2.54	122.84	118.94
25	6	307	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	c	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	4	307	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	R	605	CHL	CHD-C1D-ND	-2.54	122.12	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	608	CHL	CHB-C4A-NA	2.54	128.02	124.51
27	r	316	XAT	C35-C15-C14	-2.54	118.27	123.47
25	b	613	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
24	R	606	CHL	C3C-C4C-NC	2.54	113.42	110.57
25	5	308	CLA	C1-C2-C3	-2.54	122.64	126.75
28	n	303	NEX	C26-C27-C28	-2.54	120.63	125.99
25	b	608	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	c	601	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	c	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	q	316	CHL	CHC-C4B-NB	-2.54	121.57	124.26
24	G	313	CHL	C4-C3-C5	2.54	119.54	115.27
25	N	307	CLA	C1-C2-C3	-2.54	122.65	126.75
37	c	619	DGD	C2G-O2G-C1B	-2.54	111.55	117.79
25	8	311	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	n	307	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	3	307	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	4	314	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	2	308	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	g	301	0UR	C5-C4-C3	-2.54	123.96	127.00
24	r	307	CHL	O2D-CGD-O1D	-2.53	118.88	123.84
24	9	305	CHL	O2A-CGA-CBA	2.53	119.86	111.91
24	r	306	CHL	C4B-CHC-C1C	-2.53	120.33	126.34
25	d	404	CLA	CHB-C4A-NA	2.53	128.02	124.51
25	r	305	CLA	CHB-C4A-NA	2.53	128.02	124.51
25	D	404	CLA	C3B-C4B-NB	-2.53	108.17	110.52
25	n	307	CLA	C3B-C4B-NB	-2.53	108.17	110.52
39	D	406	PL9	C40-C39-C41	2.53	119.53	115.27
29	Y	301	0UR	C15-C14-C13	-2.53	115.32	123.22
24	r	303	CHL	C3C-C4C-NC	2.53	113.41	110.57
24	9	304	CHL	C1-C2-C3	-2.53	121.67	126.04
24	r	307	CHL	CHD-C1D-ND	-2.53	122.13	124.45
25	Y	306	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	B	606	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	V	401	8CT	C25-C24-C23	-2.53	115.32	123.22
25	N	306	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	g	317	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	C	613	8CT	C14-C15-C16	-2.53	119.31	126.42
31	b	617	8CT	C40-C12-C13	-2.53	119.38	122.92
25	4	315	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	9	308	CHL	C3B-C4B-NB	2.53	112.86	110.52
25	C	607	CLA	C3B-C4B-NB	-2.53	108.17	110.52
25	n	315	CLA	CHB-C4A-NA	2.53	128.00	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	317	CHL	CMA-C3A-C2A	-2.53	110.20	116.10
28	N	303	NEX	C26-C27-C28	-2.53	120.65	125.99
24	g	309	CHL	C3B-C4B-NB	2.53	112.86	110.52
25	A	604	CLA	C1-C2-C3	-2.53	121.67	126.04
24	p	309	CHL	C3B-C4B-NB	2.52	112.86	110.52
24	u	305	CHL	C4B-CHC-C1C	-2.52	120.35	126.34
25	b	601	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	1	308	CHL	CHC-C4B-NB	-2.52	121.59	124.26
25	B	608	CLA	CHB-C4A-NA	2.52	128.00	124.51
25	Y	313	CLA	C3B-C4B-NB	-2.52	108.17	110.52
24	5	309	CHL	CHC-C4B-NB	-2.52	121.59	124.26
24	2	306	CHL	C3C-C4C-NC	2.52	113.40	110.57
24	7	305	CHL	C3C-C4C-NC	2.52	113.40	110.57
24	1	312	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
31	c	615	8CT	C40-C12-C13	-2.52	119.39	122.92
24	1	308	CHL	C4B-CHC-C1C	-2.52	120.36	126.34
24	8	315	CHL	C4B-CHC-C1C	-2.52	120.36	126.34
32	d	409	SQD	O8-S-C6	2.52	109.76	105.74
25	1	315	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	3	308	CHL	C4B-CHC-C1C	-2.52	120.36	126.34
25	G	307	CLA	C3B-C4B-NB	-2.52	108.18	110.52
24	G	305	CHL	CHD-C1D-ND	-2.52	122.14	124.45
24	n	304	CHL	O2A-CGA-CBA	2.52	119.81	111.91
24	7	309	CHL	CHD-C4C-NC	2.52	128.17	124.20
25	1	314	CLA	CHB-C4A-NA	2.52	128.00	124.51
25	7	317	CLA	CHB-C4A-NA	2.52	128.00	124.51
25	R	612	CLA	C3B-C4B-NB	-2.52	108.18	110.52
29	G	301	0UR	C10-C9-C8	-2.52	118.32	123.47
25	p	307	CLA	C3B-C4B-NB	-2.52	108.18	110.52
24	Y	304	CHL	O2A-CGA-CBA	2.52	119.81	111.91
25	6	316	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	y	314	CLA	CMB-C2B-C1B	-2.52	121.54	125.37
25	5	308	CLA	C3B-C4B-NB	-2.52	108.18	110.52
25	3	306	CLA	CAA-C2A-C3A	-2.52	110.23	116.10
24	6	308	CHL	CHC-C4B-NB	-2.52	121.59	124.26
24	6	308	CHL	C2A-C1A-CHA	-2.52	119.46	123.86
24	q	303	CHL	C4B-CHC-C1C	-2.51	120.37	126.34
31	s	415	8CT	C39-C16-C17	-2.51	119.40	122.92
26	9	303	0IE	C17-C16-C15	2.51	122.80	118.94
25	a	604	CLA	C1-C2-C3	-2.51	121.69	126.04
25	S	610	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
25	p	316	CLA	O2D-CGD-O1D	-2.51	118.92	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	316	CLA	CHB-C4A-NA	2.51	127.99	124.51
29	2	301	0UR	C22-C16-C15	-2.51	119.40	122.92
25	7	308	CLA	C1-C2-C3	-2.51	122.69	126.75
25	8	313	CLA	CHB-C4A-NA	2.51	127.99	124.51
24	2	318	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
25	R	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	n	306	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	6	314	CLA	CAA-C2A-C3A	-2.51	110.24	116.10
24	4	305	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
24	3	312	CHL	C4B-CHC-C1C	-2.51	120.38	126.34
25	R	604	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
26	2	302	0IE	C13-C12-C11	2.51	122.79	118.94
24	p	309	CHL	C4B-CHC-C1C	-2.51	120.39	126.34
29	1	301	0UR	C22-C16-C15	-2.51	119.41	122.92
24	9	317	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
25	B	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	g	305	CHL	CHD-C1D-ND	-2.51	122.15	124.45
26	G	303	0IE	C13-C12-C11	2.51	122.79	118.94
25	C	605	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	y	312	CHL	C3C-C4C-NC	2.51	113.38	110.57
25	b	614	CLA	C3B-C4B-NB	-2.50	108.19	110.52
24	6	312	CHL	C4B-CHC-C1C	-2.50	120.40	126.34
24	y	305	CHL	O2A-CGA-CBA	2.50	119.77	111.91
25	p	316	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	7	310	CHL	C4B-CHC-C1C	-2.50	120.40	126.34
25	q	314	CLA	C3B-C4B-NB	-2.50	108.19	110.52
25	3	316	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	c	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	y	317	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	b	605	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	r	309	CHL	CHD-C1D-ND	-2.50	122.16	124.45
24	u	309	CHL	C4B-CHC-C1C	-2.50	120.41	126.34
25	s	417	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	G	308	CLA	C1-C2-C3	-2.50	122.71	126.75
32	A	609	SQD	O5-C5-C4	2.50	114.23	109.69
24	p	305	CHL	C3C-C4C-NC	2.50	113.38	110.57
24	N	304	CHL	O2A-CGA-CBA	2.50	119.75	111.91
25	d	404	CLA	C3B-C4B-NB	-2.50	108.20	110.52
24	4	317	CHL	C3B-C4B-NB	2.50	112.83	110.52
24	1	305	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
25	7	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	Y	311	CHL	C3C-C4C-NC	2.50	113.37	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	318	CHL	CHD-C1D-ND	-2.50	122.16	124.45
24	q	316	CHL	C4B-CHC-C1C	-2.50	120.42	126.34
25	p	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	p	301	0UR	C29-C30-C31	-2.50	108.90	111.74
26	5	302	0IE	C13-C12-C11	2.50	122.77	118.94
25	y	307	CLA	CHB-C4A-NA	2.50	127.96	124.51
29	y	301	0UR	C15-C14-C13	-2.50	115.43	123.22
24	g	313	CHL	C4-C3-C5	2.50	119.47	115.27
25	r	305	CLA	C3B-C4B-NB	-2.50	108.20	110.52
33	d	411	LMG	O8-C28-C29	2.50	119.74	111.91
24	8	308	CHL	C3C-C4C-NC	2.49	113.37	110.57
25	9	315	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	Y	307	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	g	301	0UR	C43-C3-C4	-2.49	122.00	125.02
25	y	308	CLA	C3B-C4B-NB	-2.49	108.20	110.52
27	r	316	XAT	C15-C14-C13	-2.49	123.75	127.31
24	9	317	CHL	C2A-C1A-CHA	-2.49	119.50	123.85
25	A	603	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	6	308	CHL	C4B-CHC-C1C	-2.49	120.42	126.34
24	9	308	CHL	C4B-CHC-C1C	-2.49	120.42	126.34
24	p	306	CHL	O2D-CGD-O1D	-2.49	118.96	123.84
25	7	307	CLA	C3B-C4B-NB	-2.49	108.20	110.52
25	C	604	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	1	310	CHL	C4A-NA-C1A	2.49	107.83	106.71
24	u	318	CHL	C3B-C4B-NB	2.49	112.83	110.52
24	y	318	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
25	B	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
31	x	601	8CT	C05-C04-C03	2.49	114.31	110.48
25	R	609	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	g	306	CHL	CHD-C1D-ND	-2.49	122.17	124.45
25	B	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	a	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	y	306	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
24	7	306	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
24	n	305	CHL	O2A-CGA-CBA	2.49	119.71	111.91
25	u	307	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	B	614	CLA	C3B-C4B-NB	-2.49	108.21	110.52
29	1	301	0UR	C29-C30-C31	-2.49	108.91	111.74
25	r	310	CLA	CHB-C4A-NA	2.48	127.95	124.51
31	S	614	8CT	C39-C16-C17	-2.48	119.44	122.92
25	9	307	CLA	CHB-C4A-NA	2.48	127.95	124.51
25	B	605	CLA	CHB-C4A-NA	2.48	127.95	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	613	8CT	C14-C15-C16	-2.48	119.44	126.42
24	7	305	CHL	O2D-CGD-O1D	-2.48	118.98	123.84
24	3	317	CHL	C4A-NA-C1A	2.48	107.82	106.71
25	2	317	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	c	616	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	4	301	0UR	C10-C9-C8	-2.48	118.39	123.47
24	1	304	CHL	C3B-C4B-NB	2.48	112.82	110.52
39	d	406	PL9	C20-C19-C21	2.48	119.44	115.27
24	4	305	CHL	CHD-C1D-ND	-2.48	122.17	124.45
29	4	301	0UR	C22-C16-C15	-2.48	119.45	122.92
24	3	305	CHL	OMC-CMC-C2C	-2.48	120.08	125.69
24	5	318	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
24	7	309	CHL	C3B-C4B-NB	2.48	112.81	110.52
25	N	307	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	4	307	CLA	CAA-C2A-C3A	-2.48	110.31	116.10
25	C	611	CLA	C3B-C4B-NB	-2.48	108.22	110.52
24	Y	317	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
32	B	618	SQD	O48-C23-C24	2.48	119.68	111.91
24	5	318	CHL	CHC-C4B-NB	-2.48	121.63	124.26
25	b	603	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
24	p	309	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
24	9	304	CHL	C4B-CHC-C1C	-2.48	120.47	126.34
25	b	606	CLA	C1-C2-C3	-2.48	121.76	126.04
24	6	310	CHL	C4B-CHC-C1C	-2.48	120.47	126.34
25	C	616	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	c	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	r	302	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
24	y	318	CHL	OBD-CAD-C3D	-2.47	122.57	128.52
25	b	612	CLA	CMB-C2B-C1B	-2.47	121.60	125.37
27	R	615	XAT	C35-C15-C14	-2.47	118.41	123.47
25	C	610	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	4	308	CHL	CHC-C4B-NB	-2.47	121.64	124.26
25	b	611	CLA	CHB-C1B-NB	2.47	126.88	124.26
24	4	312	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
25	p	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	p	310	CHL	OMC-CMC-C2C	-2.47	120.09	125.69
24	2	318	CHL	CHC-C4B-NB	-2.47	121.64	124.26
24	q	308	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
25	N	313	CLA	C1-C2-C3	-2.47	121.77	126.04
24	g	306	CHL	CHB-C4A-NA	2.47	127.93	124.51
24	q	309	CHL	C4A-NA-C1A	2.47	107.82	106.71
25	c	610	CLA	CHB-C4A-NA	2.47	127.93	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	309	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
29	1	301	0UR	C21-C12-C11	-2.47	119.46	122.92
25	S	616	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	9	306	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	C	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	6	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	b	604	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	3	310	CHL	CHC-C4B-NB	-2.47	121.64	124.26
29	7	301	0UR	C24-C25-C26	-2.47	106.92	110.30
25	4	306	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	4	316	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	1	308	CHL	C3B-C4B-NB	2.47	112.81	110.52
25	q	313	CLA	C1-C2-C3	-2.47	121.77	126.04
25	b	613	CLA	C1-C2-C3	-2.47	121.77	126.04
25	Y	316	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	p	315	CLA	O2D-CGD-CBD	2.47	115.66	111.27
25	s	410	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
32	d	409	SQD	O48-C23-C24	2.47	119.65	111.91
24	3	308	CHL	CHC-C4B-NB	-2.47	121.64	124.26
24	g	318	CHL	CMB-C2B-C1B	2.47	129.13	125.37
25	1	316	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	S	604	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	5	314	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	8	302	0IE	C6-C7-C8	2.47	122.73	118.94
25	2	317	CLA	C3B-C4B-NB	-2.47	108.23	110.52
29	5	301	0UR	C22-C16-C15	-2.47	119.47	122.92
24	n	304	CHL	C4B-CHC-C1C	-2.47	120.49	126.34
32	a	609	SQD	O6-C1-C2	2.47	112.15	108.30
32	b	618	SQD	O48-C23-C24	2.47	119.65	111.91
24	N	308	CHL	C4B-CHC-C1C	-2.47	120.49	126.34
25	1	314	CLA	CAA-C2A-C3A	-2.47	110.34	116.10
24	n	305	CHL	CHD-C1D-ND	-2.46	122.19	124.45
24	N	305	CHL	C3C-C4C-NC	2.46	113.33	110.57
24	n	305	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
25	c	606	CLA	C3B-C4B-NB	-2.46	108.23	110.52
24	9	305	CHL	C4B-CHC-C1C	-2.46	120.49	126.34
25	4	314	CLA	CAA-C2A-C3A	-2.46	110.35	116.10
29	G	301	0UR	C5-C4-C3	-2.46	124.04	127.00
24	N	305	CHL	O2A-CGA-CBA	2.46	119.64	111.91
25	3	313	CLA	CHB-C4A-NA	2.46	127.92	124.51
24	4	310	CHL	C4A-NA-C1A	2.46	107.81	106.71
39	D	406	PL9	C20-C19-C21	2.46	119.41	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	304	CHL	C4B-CHC-C1C	-2.46	120.50	126.34
24	3	317	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
24	6	310	CHL	CHC-C4B-NB	-2.46	121.65	124.26
25	1	306	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	7	314	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	C	608	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
24	N	312	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
24	n	312	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
25	g	314	CLA	CHB-C4A-NA	2.46	127.92	124.51
24	g	311	CHL	C4B-CHC-C1C	-2.46	120.50	126.34
24	s	414	CHL	CHD-C1D-ND	-2.46	122.19	124.45
24	u	309	CHL	C2A-C1A-CHA	-2.46	119.56	123.86
25	G	314	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	q	302	0IE	C6-C7-C8	2.46	122.72	118.94
24	G	313	CHL	CHC-C4B-NB	-2.46	121.65	124.26
32	D	409	SQD	C44-O6-C1	2.46	118.54	113.74
25	y	308	CLA	C1-C2-C3	-2.46	122.77	126.75
25	B	616	CLA	C3B-C4B-NB	-2.46	108.23	110.52
25	9	313	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	u	316	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	R	602	CHL	C3C-C4C-NC	2.46	113.33	110.57
25	s	405	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	p	310	CHL	C4B-CHC-C1C	-2.46	120.51	126.34
25	D	404	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	r	307	CHL	C3C-C4C-NC	2.46	113.33	110.57
29	G	301	0UR	C43-C3-C4	-2.46	122.05	125.02
24	n	305	CHL	C3C-C4C-NC	2.46	113.33	110.57
24	u	318	CHL	O2D-CGD-O1D	-2.46	119.04	123.84
26	9	302	0IE	C13-C12-C11	2.46	122.71	118.94
24	5	318	CHL	C4B-CHC-C1C	-2.46	120.52	126.34
25	9	313	CLA	C1-C2-C3	-2.46	121.80	126.04
24	Y	305	CHL	O2D-CGD-O1D	-2.45	119.04	123.84
24	6	317	CHL	O2D-CGD-O1D	-2.45	119.04	123.84
25	6	314	CLA	CHB-C4A-NA	2.45	127.91	124.51
25	b	615	CLA	CHB-C4A-NA	2.45	127.91	124.51
25	c	605	CLA	CHB-C4A-NA	2.45	127.91	124.51
24	n	308	CHL	C4B-CHC-C1C	-2.45	120.52	126.34
25	n	314	CLA	CHB-C4A-NA	2.45	127.91	124.51
25	b	602	CLA	CHB-C4A-NA	2.45	127.91	124.51
25	c	608	CLA	CHB-C4A-NA	2.45	127.91	124.51
26	9	303	0IE	C4-C5-C6	2.45	130.87	123.22
24	3	308	CHL	C2A-C1A-CHA	-2.45	119.57	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	307	CLA	CAA-C2A-C3A	-2.45	110.37	116.10
25	S	609	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
25	B	615	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	y	308	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	r	308	CHL	C4D-C3D-CAD	2.45	110.98	108.10
35	d	403	PHO	C1C-C2C-C3C	-2.45	106.57	108.61
37	c	618	DGD	C1E-O6E-C5E	-2.45	108.88	113.69
26	4	302	0IE	C13-C12-C11	2.45	122.70	118.94
24	u	318	CHL	C4B-CHC-C1C	-2.45	120.53	126.34
24	G	318	CHL	CHD-C1D-ND	-2.45	122.20	124.45
24	5	312	CHL	C3C-C4C-NC	2.45	113.32	110.57
24	p	305	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
30	4	318	LHG	O8-C23-C24	2.45	119.59	111.91
24	8	303	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
25	N	315	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	A	605	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	c	608	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
23	E	201	HEM	C4D-ND-C1D	2.45	107.60	105.07
26	y	303	0IE	C9-C10-C11	2.45	128.49	123.47
28	n	303	NEX	O24-C25-C26	-2.45	56.93	58.96
24	5	310	CHL	C3C-C4C-NC	2.45	113.31	110.57
26	g	303	0IE	C13-C12-C11	2.45	122.69	118.94
25	B	612	CLA	C1-C2-C3	-2.45	121.81	126.04
25	G	308	CLA	C3B-C4B-NB	-2.45	108.25	110.52
25	b	613	CLA	CHB-C4A-NA	2.45	127.89	124.51
24	R	601	CHL	O2D-CGD-O1D	-2.45	119.06	123.84
25	8	313	CLA	C3B-C4B-NB	-2.44	108.25	110.52
29	Y	301	0UR	C4-C5-C6	-2.44	115.59	123.22
24	2	313	CHL	C4A-NA-C1A	2.44	107.81	106.71
31	c	614	8CT	C27-C26-C28	2.44	121.93	118.08
26	u	302	0IE	C4-C3-C2	-2.44	117.98	120.08
29	2	301	0UR	C29-C30-C31	-2.44	108.96	111.74
24	8	308	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
28	6	303	NEX	O24-C25-C26	-2.44	56.94	58.96
28	s	401	NEX	O24-C25-C26	-2.44	56.94	58.96
24	u	306	CHL	C4B-CHC-C1C	-2.44	120.54	126.34
24	8	304	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
24	g	313	CHL	CHC-C4B-NB	-2.44	121.67	124.26
29	2	301	0UR	C33-C32-C31	-2.44	118.33	123.56
29	y	301	0UR	C4-C5-C6	-2.44	115.60	123.22
25	g	308	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	b	610	CLA	CHB-C4A-NA	2.44	127.89	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
24	3	317	CHL	C4B-CHC-C1C	-2.44	120.55	126.34
28	N	303	NEX	O24-C25-C26	-2.44	56.94	58.96
25	B	606	CLA	C1-C2-C3	-2.44	121.82	126.04
24	7	311	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
25	b	616	CLA	C3B-C4B-NB	-2.44	108.25	110.52
24	y	306	CHL	CHB-C4A-NA	2.44	127.89	124.51
25	R	612	CLA	CHD-C1D-ND	-2.44	122.21	124.45
24	9	317	CHL	C4B-CHC-C1C	-2.44	120.56	126.34
25	C	601	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	p	306	CHL	CHB-C1B-NB	-2.44	121.68	124.26
25	A	610	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	B	611	CLA	CHB-C1B-NB	2.44	126.84	124.26
24	2	306	CHL	CHD-C1D-ND	-2.43	122.22	124.45
26	y	302	0IE	C23-C16-C17	2.43	121.91	118.08
24	S	602	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
25	S	610	CLA	C3B-C4B-NB	-2.43	108.26	110.52
25	b	609	CLA	O2D-CGD-CBD	2.43	115.59	111.27
24	R	607	CHL	CHB-C4A-NA	2.43	127.88	124.51
24	n	311	CHL	C3C-C4C-NC	2.43	113.30	110.57
24	s	408	CHL	C3C-C4C-NC	2.43	113.30	110.57
32	D	409	SQD	O48-C23-C24	2.43	119.54	111.91
24	5	305	CHL	C4B-CHC-C1C	-2.43	120.57	126.34
25	R	610	CLA	C3B-C4B-NB	-2.43	108.26	110.52
25	7	315	CLA	O2D-CGD-CBD	2.43	115.59	111.27
24	9	310	CHL	CHC-C4B-NB	-2.43	121.68	124.26
25	u	314	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	a	605	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	2	318	CHL	C4B-CHC-C1C	-2.43	120.57	126.34
24	s	414	CHL	C3C-C4C-NC	2.43	113.30	110.57
24	Y	317	CHL	OBD-CAD-C3D	-2.43	122.67	128.52
24	7	310	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
27	R	615	XAT	C19-C9-C8	2.43	121.91	118.08
25	u	314	CLA	C1-C2-C3	-2.43	121.84	126.04
24	2	312	CHL	C3C-C4C-NC	2.43	113.30	110.57
25	N	314	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	n	304	CHL	CHC-C4B-NB	-2.43	121.69	124.26
31	T	101	8CT	C05-C04-C03	2.43	114.22	110.48
24	q	304	CHL	O2D-CGD-O1D	-2.43	119.09	123.84
29	6	301	0UR	C28-C19-C18	-2.43	109.63	112.70
25	c	601	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	4	301	0UR	C21-C12-C11	-2.43	119.52	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	u	317	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	b	614	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	1	312	CHL	C4B-CHC-C1C	-2.43	120.58	126.34
24	u	312	CHL	C4B-CHC-C1C	-2.43	120.58	126.34
24	Y	304	CHL	O2D-CGD-O1D	-2.43	119.10	123.84
25	g	308	CLA	C3B-C4B-NB	-2.43	108.27	110.52
25	s	410	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	N	305	CHL	CHD-C1D-ND	-2.42	122.23	124.45
25	B	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	B	609	CLA	O2D-CGD-CBD	2.42	115.57	111.27
25	B	612	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
32	A	609	SQD	O48-C23-C24	2.42	119.51	111.91
26	Y	302	0IE	C23-C16-C17	2.42	121.89	118.08
28	3	318	NEX	O24-C25-C26	-2.42	56.95	58.96
30	1	318	LHG	O8-C23-C24	2.42	119.50	111.91
24	Y	305	CHL	CHB-C4A-NA	2.42	127.86	124.51
24	4	308	CHL	C3B-C4B-NB	2.42	112.76	110.52
25	r	311	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	8	312	CLA	C1-C2-C3	-2.42	121.86	126.04
23	f	201	HEM	C4A-NA-C1A	2.42	107.72	105.35
24	S	607	CHL	C3C-C4C-NC	2.42	113.28	110.57
25	Y	307	CLA	C1-C2-C3	-2.42	122.84	126.75
25	B	603	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
24	G	311	CHL	C4B-CHC-C1C	-2.42	120.60	126.34
24	u	313	CHL	CHC-C4B-NB	-2.42	121.70	124.26
27	r	316	XAT	C19-C9-C8	2.42	121.89	118.08
29	G	301	0UR	C24-C25-C26	-2.42	106.99	110.30
25	u	317	CLA	C1-C2-C3	-2.42	121.86	126.04
24	q	310	CHL	CHD-C1D-ND	-2.42	122.23	124.45
24	G	318	CHL	CMB-C2B-C1B	2.42	129.05	125.37
25	q	315	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	R	607	CHL	C4D-C3D-CAD	2.42	110.94	108.10
32	a	609	SQD	O5-C5-C4	2.42	114.08	109.69
25	a	610	CLA	CHB-C4A-NA	2.42	127.85	124.51
25	c	603	CLA	CHB-C4A-NA	2.42	127.85	124.51
24	N	312	CHL	C4-C3-C5	2.42	119.34	115.27
29	G	301	0UR	C4-C5-C6	-2.42	115.68	123.22
24	6	311	CHL	C3C-C4C-NC	2.42	113.28	110.57
25	c	606	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
29	5	301	0UR	C33-C32-C31	-2.42	118.39	123.56
24	p	310	CHL	CHC-C4B-NB	-2.42	121.70	124.26
24	s	403	CHL	O2D-CGD-O1D	-2.42	119.12	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	314	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
25	Y	313	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	Y	313	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
24	3	310	CHL	C4B-CHC-C1C	-2.41	120.61	126.34
24	n	310	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
29	g	301	0UR	C4-C3-C2	-2.41	118.01	120.08
31	C	615	8CT	C35-C30-C31	2.41	115.74	111.42
25	A	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	a	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	q	303	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
29	g	301	0UR	C10-C9-C8	-2.41	118.53	123.47
29	1	301	0UR	C10-C9-C8	-2.41	118.53	123.47
24	5	311	CHL	C4B-CHC-C1C	-2.41	120.62	126.34
24	G	309	CHL	C3B-C4B-NB	2.41	112.75	110.52
24	n	317	CHL	C3B-C4B-NB	2.41	112.75	110.52
24	4	312	CHL	C4B-CHC-C1C	-2.41	120.62	126.34
25	A	610	CLA	C3B-C4B-NB	-2.41	108.28	110.52
25	u	308	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	g	310	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
25	y	314	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	u	306	CHL	OMC-CMC-C2C	-2.41	120.24	125.69
24	S	601	CHL	C3C-C4C-NC	2.41	113.27	110.57
24	9	305	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
32	d	409	SQD	C44-O6-C1	2.41	118.44	113.74
24	9	304	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
25	B	613	CLA	C1-C2-C3	-2.41	121.88	126.04
24	S	613	CHL	C3C-C4C-NC	2.41	113.27	110.57
25	2	314	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	S	609	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	a	610	CLA	C3B-C4B-NB	-2.41	108.28	110.52
24	5	306	CHL	CHD-C1D-ND	-2.41	122.24	124.45
26	1	302	0IE	C13-C12-C11	2.41	122.63	118.94
25	G	308	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	n	312	CHL	C4-C3-C5	2.41	119.32	115.27
24	1	305	CHL	C3C-C4C-NC	2.40	113.27	110.57
25	b	612	CLA	C1-C2-C3	-2.40	121.88	126.04
24	9	311	CHL	C4B-CHC-C1C	-2.40	120.64	126.34
25	4	307	CLA	CHB-C4A-NA	2.40	127.84	124.51
24	2	310	CHL	CHD-C1D-ND	-2.40	122.25	124.45
25	r	305	CLA	CMA-C3A-C2A	-2.40	110.49	116.10
24	n	310	CHL	C4B-CHC-C1C	-2.40	120.64	126.34
24	9	312	CHL	CHC-C4B-NB	-2.40	121.71	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	314	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	6	305	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
24	r	302	CHL	C4B-CHC-C1C	-2.40	120.64	126.34
24	6	311	CHL	CHD-C1D-ND	-2.40	122.25	124.45
25	g	308	CLA	C1-C2-C3	-2.40	122.87	126.75
24	N	310	CHL	C4B-CHC-C1C	-2.40	120.64	126.34
24	9	304	CHL	C4A-NA-C1A	2.40	107.78	106.71
24	q	304	CHL	CMB-C2B-C1B	2.40	129.02	125.37
24	2	310	CHL	C3C-C4C-NC	2.40	113.26	110.57
24	r	308	CHL	CHB-C4A-NA	2.40	127.83	124.51
25	5	307	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	u	313	CHL	C4B-CHC-C1C	-2.40	120.65	126.34
25	C	606	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
24	G	312	CHL	C5-C3-C4	2.40	119.90	114.60
24	Y	308	CHL	C4B-CHC-C1C	-2.40	120.65	126.34
28	r	301	NEX	O24-C25-C26	-2.40	56.97	58.96
25	C	601	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	y	315	CLA	C3B-C4B-NB	-2.40	108.29	110.52
24	R	601	CHL	C4B-CHC-C1C	-2.40	120.65	126.34
24	R	606	CHL	CHD-C1D-ND	-2.40	122.25	124.45
24	N	311	CHL	C3C-C4C-NC	2.40	113.26	110.57
25	N	316	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	C	606	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	8	305	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	p	302	0IE	C20-C3-C4	-2.39	121.75	124.83
23	E	201	HEM	C4A-NA-C1A	2.39	107.69	105.35
24	q	310	CHL	CHB-C4A-NA	2.39	127.82	124.51
31	X	601	8CT	C22-C21-C23	2.39	121.85	118.08
24	y	305	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
25	B	614	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	6	302	0IE	C13-C12-C11	2.39	122.61	118.94
24	8	310	CHL	CMB-C2B-C1B	2.39	129.01	125.37
25	s	411	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	2	309	CHL	CHC-C4B-NB	-2.39	121.72	124.26
31	C	614	8CT	C27-C26-C28	2.39	121.85	118.08
25	s	411	CLA	C3B-C4B-NB	-2.39	108.30	110.52
24	S	602	CHL	CHB-C4A-NA	2.39	127.82	124.51
24	G	310	CHL	C4B-CHC-C1C	-2.39	120.67	126.34
24	5	310	CHL	CHD-C1D-ND	-2.39	122.26	124.45
26	u	303	0IE	C17-C16-C15	2.39	122.61	118.94
35	D	403	PHO	C1C-C2C-C3C	-2.39	106.62	108.61
32	b	618	SQD	C3-C4-C5	2.39	114.50	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	318	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
24	N	304	CHL	CHC-C4B-NB	-2.39	121.73	124.26
24	N	310	CHL	CHC-C4B-NB	-2.39	121.73	124.26
25	r	311	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	7	308	CLA	C3B-C4B-NB	-2.39	108.30	110.52
24	n	317	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
25	b	609	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	2	305	CHL	C4B-CHC-C1C	-2.39	120.68	126.34
24	g	313	CHL	C4B-CHC-C1C	-2.39	120.68	126.34
24	y	309	CHL	C4A-NA-C1A	2.39	107.78	106.71
31	S	615	8CT	C18-C19-C20	-2.39	118.58	123.47
25	n	316	CLA	C3B-C4B-NB	-2.39	108.30	110.52
25	9	316	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	g	310	CHL	C4B-CHC-C1C	-2.39	120.68	126.34
24	3	311	CHL	CHC-C4B-NB	-2.39	121.73	124.26
26	2	302	0IE	C4-C3-C2	-2.39	118.03	120.08
26	7	302	0IE	C20-C3-C4	-2.39	121.76	124.83
24	9	317	CHL	C3B-C4B-NB	2.39	112.73	110.52
29	g	301	0UR	C24-C25-C26	-2.39	107.04	110.30
25	r	311	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
25	q	305	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	N	310	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
31	x	601	8CT	C27-C26-C28	2.38	121.83	118.08
24	2	311	CHL	C4B-CHC-C1C	-2.38	120.69	126.34
24	G	310	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
24	8	307	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
25	6	306	CLA	CHB-C4A-NA	2.38	127.81	124.51
31	X	601	8CT	C27-C26-C28	2.38	121.83	118.08
24	s	402	CHL	C3C-C4C-NC	2.38	113.24	110.57
24	9	312	CHL	C4B-CHC-C1C	-2.38	120.69	126.34
25	b	610	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	n	314	CLA	C3B-C4B-NB	-2.38	108.31	110.52
24	1	309	CHL	C4B-CHC-C1C	-2.38	120.69	126.34
24	R	607	CHL	CHD-C1D-ND	-2.38	122.27	124.45
31	v	401	8CT	C11-C10-C03	-2.38	120.51	127.20
24	q	304	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
25	g	315	CLA	C3B-C4B-NB	-2.38	108.31	110.52
24	N	311	CHL	CHD-C1D-ND	-2.38	122.27	124.45
24	8	304	CHL	CMB-C2B-C1B	2.38	129.00	125.37
25	3	306	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	4	309	CHL	C4B-CHC-C1C	-2.38	120.69	126.34
25	B	612	CLA	CHB-C4A-NA	2.38	127.80	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	302	0IE	C13-C12-C11	2.38	122.59	118.94
24	g	312	CHL	C5-C3-C4	2.38	119.86	114.60
24	s	409	CHL	CHB-C4A-NA	2.38	127.80	124.51
25	B	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	u	310	CHL	C4B-CHC-C1C	-2.38	120.70	126.34
24	S	608	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
31	c	615	8CT	C35-C30-C31	2.38	115.67	111.42
24	g	306	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
24	G	306	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
24	s	409	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
23	f	201	HEM	C4D-ND-C1D	2.37	107.53	105.07
25	7	308	CLA	CHB-C4A-NA	2.37	127.80	124.51
24	u	306	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
24	q	308	CHL	CHD-C1D-ND	-2.37	122.27	124.45
24	2	310	CHL	C4B-CHC-C1C	-2.37	120.71	126.34
24	Y	312	CHL	C4-C3-C5	2.37	119.26	115.27
25	C	601	CLA	CMB-C2B-C1B	-2.37	121.75	125.37
26	p	303	0IE	C17-C16-C15	2.37	122.58	118.94
24	g	306	CHL	C3C-C4C-NC	2.37	113.23	110.57
31	V	401	8CT	C11-C10-C03	-2.37	120.54	127.20
25	C	603	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	y	313	CHL	C4-C3-C5	2.37	119.26	115.27
25	c	601	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
24	7	310	CHL	C3B-C4B-NB	2.37	112.72	110.52
24	8	304	CHL	OMC-CMC-C2C	-2.37	120.33	125.69
24	7	306	CHL	C4B-CHC-C1C	-2.37	120.71	126.34
24	r	307	CHL	C4A-NA-C1A	2.37	107.77	106.71
24	G	313	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
25	s	413	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	7	318	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
29	g	301	0UR	C4-C5-C6	-2.37	115.82	123.22
25	S	610	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	g	315	CLA	CHB-C4A-NA	2.37	127.79	124.51
32	D	409	SQD	O5-C5-C4	2.37	114.00	109.69
31	T	101	8CT	C40-C12-C13	-2.37	119.61	122.92
25	Y	307	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
25	N	316	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	u	305	CHL	C1-C2-C3	-2.37	121.95	126.04
24	6	305	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
24	6	310	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
26	N	302	0IE	C13-C12-C11	2.37	122.57	118.94
26	n	302	0IE	C13-C12-C11	2.37	122.57	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	316	CLA	CHB-C1B-NB	2.37	126.76	124.26
26	4	302	0IE	C23-C16-C17	2.36	121.80	118.08
26	1	302	0IE	C23-C16-C17	2.36	121.80	118.08
24	3	305	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
25	n	316	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	n	313	CLA	C1-C2-C3	-2.36	121.95	126.04
25	8	311	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
32	d	409	SQD	O5-C5-C4	2.36	113.98	109.69
25	R	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	2	307	CLA	CHB-C4A-NA	2.36	127.78	124.51
29	u	301	0UR	C24-C25-C26	-2.36	107.07	110.30
26	q	302	0IE	C13-C12-C11	2.36	122.56	118.94
31	x	601	8CT	C22-C21-C23	2.36	121.80	118.08
24	s	406	CHL	C4B-CHC-C1C	-2.36	120.74	126.34
24	6	309	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
24	Y	305	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
24	9	308	CHL	C2A-C1A-CHA	-2.36	119.73	123.86
24	R	608	CHL	C4A-NA-C1A	2.36	107.77	106.71
24	s	414	CHL	CMA-C3A-C2A	-2.36	110.59	116.10
24	g	318	CHL	C4B-CHC-C1C	-2.36	120.74	126.34
29	6	301	0UR	C10-C9-C8	-2.36	118.64	123.47
24	r	308	CHL	CHD-C1D-ND	-2.36	122.29	124.45
24	n	308	CHL	CHC-C4B-NB	-2.36	121.76	124.26
25	N	307	CLA	C3B-C4B-NB	-2.36	108.33	110.52
26	7	303	0IE	C17-C16-C15	2.36	122.56	118.94
37	c	619	DGD	O1G-C1A-O1A	-2.36	117.64	123.59
24	q	311	CHL	CMB-C2B-C1B	2.36	128.96	125.37
24	s	402	CHL	CHD-C1D-ND	-2.36	122.29	124.45
31	D	410	8CT	C19-C18-C17	-2.36	118.65	123.47
24	8	307	CHL	C4B-CHC-C1C	-2.36	120.75	126.34
29	8	301	0UR	C15-C14-C13	-2.35	115.87	123.22
24	2	313	CHL	C4B-CHC-C1C	-2.35	120.76	126.34
24	S	601	CHL	CHD-C1D-ND	-2.35	122.29	124.45
24	S	605	CHL	C4B-CHC-C1C	-2.35	120.76	126.34
24	S	607	CHL	CHD-C1D-ND	-2.35	122.29	124.45
26	N	302	0IE	C23-C16-C17	2.35	121.78	118.08
24	y	309	CHL	C4B-CHC-C1C	-2.35	120.76	126.34
25	y	317	CLA	CHB-C1B-NB	2.35	126.75	124.26
25	C	606	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	5	313	CHL	C4B-CHC-C1C	-2.35	120.76	126.34
30	c	617	LHG	O8-C23-C24	2.35	119.28	111.91
24	q	304	CHL	C3C-C4C-NC	2.35	113.21	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	311	CLA	C1-C2-C3	-2.35	121.98	126.04
25	B	610	CLA	CHB-C1B-NB	2.35	126.75	124.26
25	A	605	CLA	CHB-C1B-NB	2.35	126.75	124.26
25	4	306	CLA	C3B-C4B-NB	-2.35	108.33	110.52
24	1	304	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
30	C	617	LHG	O8-C23-C24	2.35	119.28	111.91
26	5	302	0IE	C4-C3-C2	-2.35	118.06	120.08
32	A	609	SQD	C1-O5-C5	2.35	118.30	113.69
24	4	317	CHL	C2A-C1A-CHA	-2.35	119.75	123.85
24	p	306	CHL	C4B-CHC-C1C	-2.35	120.77	126.34
24	S	613	CHL	CMA-C3A-C2A	-2.35	110.62	116.10
24	5	306	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
25	b	612	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	1	307	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	3	312	CHL	CHC-C4B-NB	-2.35	121.77	124.26
31	t	101	8CT	C05-C04-C03	2.35	114.09	110.48
24	q	309	CHL	C3C-C4C-NC	2.35	113.20	110.57
24	1	317	CHL	C2A-C1A-CHA	-2.35	119.76	123.85
24	6	317	CHL	C4B-CHC-C1C	-2.35	120.77	126.34
25	c	606	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	s	416	8CT	C18-C19-C20	-2.35	118.67	123.47
24	6	312	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
31	t	101	8CT	C40-C12-C13	-2.35	119.64	122.92
25	B	609	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	u	310	CHL	O2D-CGD-O1D	-2.34	119.25	123.84
24	4	309	CHL	O2D-CGD-O1D	-2.34	119.25	123.84
24	u	311	CHL	O2D-CGD-O1D	-2.34	119.25	123.84
24	1	305	CHL	CHD-C1D-ND	-2.34	122.30	124.45
24	8	315	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
24	1	309	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
24	6	304	CHL	C4B-CHC-C1C	-2.34	120.78	126.34
24	3	312	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
24	4	305	CHL	C3C-C4C-NC	2.34	113.20	110.57
26	u	302	0IE	C13-C12-C11	2.34	122.53	118.94
25	p	308	CLA	C3B-C4B-NB	-2.34	108.34	110.52
24	u	311	CHL	CHC-C4B-NB	-2.34	121.78	124.26
24	8	309	CHL	CHD-C1D-ND	-2.34	122.30	124.45
24	N	317	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
25	Y	314	CLA	C3B-C4B-NB	-2.34	108.34	110.52
24	3	309	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
25	a	607	CLA	C1-C2-C3	-2.34	122.00	126.04
25	G	307	CLA	CHB-C4A-NA	2.34	127.75	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	619	LMG	O7-C10-O9	-2.34	118.05	123.70
24	9	310	CHL	C4B-CHC-C1C	-2.34	120.79	126.34
24	G	318	CHL	C4B-CHC-C1C	-2.34	120.79	126.34
25	y	308	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
25	C	609	CLA	CHB-C1B-NB	2.34	126.73	124.26
25	g	307	CLA	CHB-C4A-NA	2.34	127.74	124.51
24	3	310	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
24	2	306	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
24	4	304	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
24	4	310	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
27	r	316	XAT	C4-C3-C2	-2.33	106.26	110.77
37	C	620	DGD	O1G-C1A-O1A	-2.33	117.70	123.59
24	1	310	CHL	O2D-CGD-O1D	-2.33	119.27	123.84
24	2	311	CHL	CHC-C4B-NB	-2.33	121.79	124.26
24	g	311	CHL	CHC-C4B-NB	-2.33	121.79	124.26
25	a	605	CLA	CHB-C1B-NB	2.33	126.73	124.26
29	5	301	0UR	C29-C30-C31	-2.33	109.08	111.74
24	4	311	CHL	CHC-C4B-NB	-2.33	121.79	124.26
25	3	314	CLA	CAA-C2A-C3A	-2.33	110.65	116.10
25	8	311	CLA	CHB-C1B-NB	2.33	126.73	124.26
26	p	302	0IE	C5-C4-C3	2.33	129.81	127.00
25	s	404	CLA	CHB-C4A-NA	2.33	127.73	124.51
24	g	305	CHL	C4B-CHC-C1C	-2.33	120.81	126.34
24	N	317	CHL	C3B-C4B-NB	2.33	112.68	110.52
31	B	617	8CT	C18-C19-C20	-2.33	118.70	123.47
24	4	309	CHL	C4A-NA-C1A	2.33	107.75	106.71
29	p	301	0UR	C24-C25-C26	-2.33	107.12	110.30
24	6	311	CHL	CHC-C4B-NB	-2.33	121.79	124.26
24	8	304	CHL	C3C-C4C-NC	2.33	113.18	110.57
24	1	308	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
24	r	306	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
25	8	312	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	S	604	CLA	C3B-C4B-NB	-2.33	108.36	110.52
24	y	318	CHL	C4B-CHC-C1C	-2.33	120.82	126.34
26	u	302	0IE	C6-C7-C8	2.33	122.51	118.94
24	n	305	CHL	C4B-CHC-C1C	-2.33	120.82	126.34
25	A	610	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
25	a	610	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
24	2	313	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
24	u	309	CHL	O2D-CGD-O1D	-2.32	119.29	123.84
26	7	302	0IE	C5-C4-C3	2.32	129.80	127.00
26	8	302	0IE	C13-C12-C11	2.32	122.51	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	313	CHL	C4B-CHC-C1C	-2.32	120.83	126.34
25	G	315	CLA	CHB-C4A-NA	2.32	127.73	124.51
31	T	101	8CT	C39-C16-C17	-2.32	119.67	122.92
32	B	618	SQD	C3-C4-C5	2.32	114.38	110.24
25	b	602	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	7	301	0UR	C10-C9-C8	-2.32	118.72	123.47
24	5	310	CHL	C4B-CHC-C1C	-2.32	120.83	126.34
24	4	308	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
24	y	306	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
24	r	309	CHL	C3C-C4C-NC	2.32	113.17	110.57
29	u	301	0UR	C28-C19-C18	-2.32	109.77	112.70
24	N	309	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
25	p	308	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	4	301	0UR	C29-C30-C31	-2.32	109.10	111.74
24	6	309	CHL	C5-C3-C4	2.32	119.73	114.60
24	g	313	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
26	y	303	0IE	C13-C12-C11	2.32	122.50	118.94
24	S	601	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
24	g	312	CHL	C4A-NA-C1A	2.32	107.75	106.71
25	q	312	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
24	8	308	CHL	CHD-C1D-ND	-2.32	122.32	124.45
25	B	602	CLA	C3B-C4B-NB	-2.32	108.36	110.52
25	B	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	6	312	CHL	CHC-C4B-NB	-2.32	121.80	124.26
26	Y	303	0IE	C13-C12-C11	2.32	122.50	118.94
24	n	311	CHL	CHD-C1D-ND	-2.32	122.33	124.45
24	u	313	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
24	u	305	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
24	s	402	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
25	q	313	CLA	CHB-C4A-NA	2.32	127.71	124.51
24	Y	317	CHL	C4B-CHC-C1C	-2.31	120.85	126.34
24	7	305	CHL	CHD-C1D-ND	-2.31	122.33	124.45
24	R	605	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
29	q	301	0UR	C15-C14-C13	-2.31	116.00	123.22
24	9	310	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
24	y	313	CHL	C4B-CHC-C1C	-2.31	120.85	126.34
24	5	313	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
25	5	314	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
24	9	309	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
25	b	612	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
24	4	304	CHL	C2A-C1A-CHA	-2.31	119.82	123.85
24	Y	319	CHL	C3C-C4C-NC	2.31	113.16	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	316	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
33	D	401	LMG	O6-C1-C2	-2.31	105.46	110.35
33	d	401	LMG	O6-C1-C2	-2.31	105.46	110.35
24	1	304	CHL	C2A-C1A-CHA	-2.31	119.82	123.85
25	B	610	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
24	u	311	CHL	C4B-CHC-C1C	-2.31	120.86	126.34
24	n	310	CHL	CHC-C4B-NB	-2.31	121.81	124.26
25	N	314	CLA	C1-C2-C3	-2.31	122.05	126.04
24	S	601	CHL	C4B-CHC-C1C	-2.31	120.86	126.34
25	A	607	CLA	C1-C2-C3	-2.31	122.05	126.04
24	7	306	CHL	CHB-C1B-NB	-2.31	121.81	124.26
25	3	313	CLA	CMA-C3A-C2A	-2.31	110.72	116.10
25	S	612	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	p	309	CHL	C2A-C1A-CHA	-2.31	119.83	123.86
24	7	310	CHL	CHC-C4B-NB	-2.30	121.82	124.26
25	q	312	CLA	C1-C2-C3	-2.30	122.06	126.04
24	q	307	CHL	C4B-CHC-C1C	-2.30	120.87	126.34
28	9	319	NEX	C39-C29-C30	-2.30	119.70	122.92
25	1	306	CLA	C3B-C4B-NB	-2.30	108.38	110.52
24	s	402	CHL	C4B-CHC-C1C	-2.30	120.88	126.34
24	q	303	CHL	CHC-C4B-NB	-2.30	121.82	124.26
24	9	312	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
28	n	303	NEX	C35-C15-C14	-2.30	118.76	123.47
25	2	314	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
24	p	310	CHL	C3B-C4B-NB	2.30	112.65	110.52
24	8	303	CHL	CHC-C4B-NB	-2.30	121.82	124.26
24	G	305	CHL	C4B-CHC-C1C	-2.30	120.89	126.34
24	N	305	CHL	C4B-CHC-C1C	-2.30	120.89	126.34
24	n	309	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
25	S	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
31	X	601	8CT	C04-C03-C02	-2.30	119.38	122.61
24	3	311	CHL	C3C-C4C-NC	2.30	113.15	110.57
24	r	309	CHL	C4A-NA-C1A	2.30	107.74	106.71
24	9	308	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
24	N	312	CHL	C4B-CHC-C1C	-2.30	120.89	126.34
39	D	406	PL9	C31-C32-C33	-2.30	104.33	111.88
25	c	609	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	B	603	CLA	C3B-C4B-NB	-2.30	108.39	110.52
25	b	603	CLA	C3B-C4B-NB	-2.30	108.39	110.52
25	s	405	CLA	C3B-C4B-NB	-2.30	108.39	110.52
25	p	314	CLA	C1-C2-C3	-2.30	122.07	126.04
29	8	301	0UR	C10-C9-C8	-2.29	118.77	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	314	CLA	C1-C2-C3	-2.29	122.08	126.04
28	u	304	NEX	C39-C29-C30	-2.29	119.71	122.92
28	p	304	NEX	C39-C29-C30	-2.29	119.71	122.92
25	8	306	CLA	C3B-C4B-NB	-2.29	108.39	110.52
28	6	303	NEX	C35-C15-C14	-2.29	118.78	123.47
24	3	309	CHL	C5-C3-C4	2.29	119.67	114.60
31	X	601	8CT	C35-C30-C31	2.29	115.52	111.42
31	S	615	8CT	C40-C12-C13	-2.29	119.71	122.92
29	y	301	0UR	C10-C9-C8	-2.29	118.78	123.47
24	G	311	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
26	7	302	0IE	C13-C12-C11	2.29	122.46	118.94
24	y	313	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
25	G	315	CLA	C1-C2-C3	-2.29	122.08	126.04
24	G	306	CHL	C3C-C4C-NC	2.29	113.14	110.57
31	t	101	8CT	C39-C16-C17	-2.29	119.72	122.92
24	G	309	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
28	s	401	NEX	C35-C15-C14	-2.29	118.79	123.47
24	N	309	CHL	CHD-C1D-ND	-2.29	122.35	124.45
24	Y	317	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
29	5	301	0UR	C10-C9-C8	-2.29	118.79	123.47
25	r	314	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	n	309	CHL	CHA-C1A-NA	2.29	131.63	126.40
29	9	301	0UR	C28-C19-C18	-2.29	109.81	112.70
24	s	408	CHL	CHD-C1D-ND	-2.29	122.35	124.45
24	u	312	CHL	CHC-C4B-NB	-2.28	121.84	124.26
24	8	310	CHL	O2D-CGD-O1D	-2.28	119.37	123.84
25	G	315	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	a	608	8CT	C28-C26-C25	-2.28	115.44	118.94
24	g	310	CHL	CHC-C4B-NB	-2.28	121.84	124.26
25	1	313	CLA	C1-C2-C3	-2.28	122.09	126.04
25	n	314	CLA	C1-C2-C3	-2.28	122.09	126.04
25	b	604	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	p	311	CHL	C4B-CHC-C1C	-2.28	120.92	126.34
25	R	613	CLA	CHB-C4A-NA	2.28	127.67	124.51
31	b	617	8CT	C22-C21-C20	-2.28	119.72	122.92
39	d	406	PL9	C31-C32-C33	-2.28	104.38	111.88
25	b	610	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
26	r	315	0IE	C23-C16-C17	2.28	121.67	118.08
25	r	313	CLA	CHD-C1D-ND	-2.28	122.36	124.45
24	G	306	CHL	OMC-CMC-C2C	-2.28	120.53	125.69
24	Y	311	CHL	CHD-C1D-ND	-2.28	122.36	124.45
24	y	312	CHL	CHD-C1D-ND	-2.28	122.36	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	312	CHL	C4B-CHC-C1C	-2.28	120.93	126.34
29	3	301	0UR	C43-C3-C4	-2.28	122.26	125.02
25	3	314	CLA	CHB-C4A-NA	2.28	127.66	124.51
29	p	301	0UR	C23-C24-C25	-2.28	108.50	113.64
24	G	312	CHL	C4B-CHC-C1C	-2.28	120.93	126.34
28	N	303	NEX	C35-C15-C14	-2.28	118.81	123.47
29	Y	301	0UR	C10-C9-C8	-2.28	118.81	123.47
28	r	301	NEX	C35-C15-C14	-2.28	118.81	123.47
24	y	312	CHL	C5-C3-C4	2.28	119.63	114.60
24	2	311	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
24	4	317	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
28	7	304	NEX	C39-C29-C30	-2.28	119.73	122.92
24	2	312	CHL	CHD-C1D-ND	-2.28	122.36	124.45
25	N	314	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	d	410	8CT	C19-C18-C17	-2.28	118.81	123.47
28	4	303	NEX	C39-C29-C30	-2.28	119.74	122.92
25	y	314	CLA	CHB-C1B-NB	2.27	126.67	124.26
24	r	307	CHL	C4B-CHC-C1C	-2.27	120.94	126.34
25	C	611	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
24	9	309	CHL	C4B-CHC-C1C	-2.27	120.94	126.34
28	5	304	NEX	C39-C29-C30	-2.27	119.74	122.92
28	y	304	NEX	C39-C29-C30	-2.27	119.74	122.92
31	t	101	8CT	C27-C26-C25	-2.27	119.74	122.92
25	g	315	CLA	C1-C2-C3	-2.27	122.11	126.04
31	x	601	8CT	C35-C30-C31	2.27	115.49	111.42
31	c	614	8CT	C40-C12-C13	-2.27	119.74	122.92
25	b	603	CLA	CHB-C4A-NA	2.27	127.65	124.51
24	p	305	CHL	CHD-C1D-ND	-2.27	122.37	124.45
30	C	617	LHG	C26-C25-C24	2.27	121.35	113.19
24	q	307	CHL	O2D-CGD-O1D	-2.27	119.40	123.84
24	7	306	CHL	CHB-C1B-C2B	-2.27	120.83	127.24
24	1	317	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
25	N	313	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
28	3	318	NEX	C35-C15-C14	-2.27	118.83	123.47
24	y	311	CHL	CHD-C1D-ND	-2.27	122.37	124.45
29	1	301	0UR	C33-C32-C31	-2.27	118.71	123.56
29	p	301	0UR	C10-C9-C8	-2.27	118.83	123.47
28	2	304	NEX	C39-C29-C30	-2.27	119.75	122.92
24	3	308	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
24	5	311	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
26	p	302	0IE	C23-C16-C17	2.27	121.65	118.08
28	r	317	NEX	C39-C29-C30	-2.27	119.75	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	301	0UR	C10-C9-C8	-2.26	118.83	123.47
31	C	614	8CT	C40-C12-C13	-2.26	119.75	122.92
24	Y	312	CHL	OMC-CMC-C2C	-2.26	120.57	125.69
24	6	317	CHL	C2A-C3A-C4A	-2.26	98.90	101.78
31	x	601	8CT	C40-C12-C13	-2.26	119.75	122.92
25	B	612	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
25	c	611	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
30	c	617	LHG	C26-C25-C24	2.26	121.32	113.19
28	R	616	NEX	C39-C29-C30	-2.26	119.75	122.92
25	p	317	CLA	O2D-CGD-CBD	2.26	115.29	111.27
28	S	617	NEX	C39-C29-C30	-2.26	119.76	122.92
24	p	313	CHL	C4B-CHC-C1C	-2.26	120.98	126.34
25	q	312	CLA	CHB-C1B-NB	2.26	126.65	124.26
24	y	318	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
28	1	303	NEX	C39-C29-C30	-2.26	119.76	122.92
29	7	301	0UR	C15-C14-C13	-2.26	116.17	123.22
24	p	311	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
24	q	311	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
31	c	613	8CT	C25-C24-C23	-2.26	116.17	123.22
27	R	615	XAT	C4-C3-C2	-2.26	106.41	110.77
31	A	608	8CT	C28-C26-C25	-2.26	115.47	118.94
24	Y	309	CHL	C4D-C3D-CAD	2.26	110.76	108.10
29	p	301	0UR	C15-C14-C13	-2.26	116.17	123.22
24	n	304	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
24	g	309	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
24	y	311	CHL	C4B-CHC-C1C	-2.26	120.98	126.34
25	C	606	CLA	CHB-C1B-NB	2.26	126.65	124.26
24	s	414	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
25	r	304	CLA	C3B-C4B-NB	-2.26	108.42	110.52
25	7	317	CLA	O2D-CGD-CBD	2.26	115.28	111.27
25	B	604	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	2	305	CHL	O2D-CGD-O1D	-2.26	119.43	123.84
24	N	305	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
24	7	312	CHL	C4B-CHC-C1C	-2.25	121.00	126.34
24	p	306	CHL	CHB-C1B-C2B	-2.25	120.88	127.24
24	Y	311	CHL	C5-C3-C4	2.25	119.57	114.60
24	6	308	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
31	a	608	8CT	C40-C12-C13	-2.25	119.77	122.92
25	c	605	CLA	CHB-C1B-NB	2.25	126.64	124.26
28	r	317	NEX	C31-C32-C33	-2.25	120.10	126.42
25	C	605	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
24	8	309	CHL	O2D-CGD-O1D	-2.25	119.44	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	303	0IE	C4-C5-C6	2.25	130.23	123.22
29	1	301	0UR	C24-C25-C26	-2.25	107.23	110.30
32	B	618	SQD	C44-O6-C1	2.25	118.13	113.74
26	R	614	0IE	C23-C16-C17	2.25	121.62	118.08
26	7	302	0IE	C23-C16-C17	2.25	121.62	118.08
25	B	611	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
24	p	318	CHL	C4B-CHC-C1C	-2.25	121.01	126.34
24	5	312	CHL	CHD-C1D-ND	-2.24	122.39	124.45
24	Y	311	CHL	C4B-CHC-C1C	-2.24	121.01	126.34
25	B	616	CLA	CHC-C4B-NB	2.24	126.63	124.26
24	n	312	CHL	C4B-CHC-C1C	-2.24	121.02	126.34
24	7	311	CHL	C4B-CHC-C1C	-2.24	121.02	126.34
24	S	613	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
24	Y	304	CHL	CHD-C1D-ND	-2.24	122.39	124.45
28	G	304	NEX	C39-C29-C30	-2.24	119.78	122.92
24	5	311	CHL	CHC-C4B-NB	-2.24	121.88	124.26
24	N	308	CHL	CHC-C4B-NB	-2.24	121.88	124.26
25	D	404	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
29	G	301	0UR	C15-C14-C13	-2.24	116.22	123.22
26	9	302	0IE	C5-C4-C3	2.24	129.70	127.00
24	p	311	CHL	CHC-C4B-NB	-2.24	121.89	124.26
26	p	302	0IE	C13-C12-C11	2.24	122.38	118.94
25	C	601	CLA	C2D-C1D-ND	-2.24	108.45	110.10
25	R	603	CLA	C3B-C4B-NB	-2.24	108.44	110.52
24	5	305	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	q	310	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
26	N	302	0IE	C5-C4-C3	2.24	129.70	127.00
25	A	603	CLA	CMB-C2B-C3B	2.24	132.01	126.59
24	R	608	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	6	304	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
25	r	313	CLA	C3B-C4B-NB	-2.24	108.44	110.52
24	y	305	CHL	CHD-C1D-ND	-2.24	122.40	124.45
31	c	613	8CT	C06-C07-C02	-2.24	110.08	114.08
24	n	309	CHL	C4D-C3D-CAD	2.24	110.73	108.10
25	c	605	CLA	CMB-C2B-C1B	-2.24	121.97	125.37
24	r	309	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
24	G	305	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
29	y	301	0UR	C24-C25-C26	-2.23	107.25	110.30
24	Y	310	CHL	C4B-CHC-C1C	-2.23	121.04	126.34
24	7	310	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
28	R	616	NEX	C31-C32-C33	-2.23	120.14	126.42
25	a	603	CLA	CMB-C2B-C3B	2.23	132.00	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	309	CHL	CHA-C1A-NA	2.23	131.51	126.40
24	G	310	CHL	CHC-C4B-NB	-2.23	121.89	124.26
25	b	611	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
24	g	306	CHL	OMC-CMC-C2C	-2.23	120.64	125.69
31	s	416	8CT	C40-C12-C13	-2.23	119.80	122.92
29	N	301	0UR	C10-C9-C8	-2.23	118.90	123.47
32	b	618	SQD	C44-O6-C1	2.23	118.10	113.74
24	4	310	CHL	CHC-C4B-NB	-2.23	121.89	124.26
25	b	607	CLA	CHB-C1B-NB	2.23	126.62	124.26
31	s	416	8CT	C11-C10-C03	-2.23	120.94	127.20
24	8	307	CHL	C4A-NA-C1A	2.23	107.71	106.71
29	q	301	0UR	C10-C9-C8	-2.23	118.90	123.47
33	w	201	LMG	O7-C10-O9	-2.23	118.31	123.70
25	B	609	CLA	C3B-C4B-NB	-2.23	108.45	110.52
24	7	313	CHL	C4B-CHC-C1C	-2.23	121.05	126.34
25	B	606	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
25	d	404	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
24	1	310	CHL	CHC-C4B-NB	-2.23	121.90	124.26
24	9	311	CHL	CHC-C4B-NB	-2.23	121.90	124.26
25	R	610	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
24	7	309	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
24	3	304	CHL	C4B-CHC-C1C	-2.23	121.05	126.34
24	R	608	CHL	C4B-CHC-C1C	-2.23	121.05	126.34
29	n	301	0UR	C10-C9-C8	-2.23	118.91	123.47
24	y	309	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
24	7	318	CHL	C4B-CHC-C1C	-2.23	121.06	126.34
25	d	404	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
25	b	606	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
24	y	312	CHL	C4B-CHC-C1C	-2.23	121.06	126.34
24	s	409	CHL	C4B-CHC-C1C	-2.23	121.06	126.34
24	p	310	CHL	O2D-CGD-O1D	-2.23	119.49	123.84
28	u	304	NEX	C31-C32-C33	-2.23	120.17	126.42
28	5	304	NEX	C31-C32-C33	-2.22	120.17	126.42
24	S	608	CHL	C4B-CHC-C1C	-2.22	121.06	126.34
25	Y	314	CLA	CHB-C4A-NA	2.22	127.59	124.51
25	8	306	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	6	304	CHL	C4A-NA-C1A	2.22	107.71	106.71
25	N	307	CLA	CHD-C1D-ND	-2.22	122.41	124.45
24	R	605	CHL	C4B-CHC-C1C	-2.22	121.06	126.34
25	7	314	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	1	311	CHL	CHC-C4B-NB	-2.22	121.90	124.26
24	q	304	CHL	CHC-C4B-NB	-2.22	121.91	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	607	CLA	CHB-C1B-NB	2.22	126.61	124.26
24	g	305	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
25	q	313	CLA	C3B-C4B-NB	-2.22	108.45	110.52
27	R	615	XAT	C38-C25-C24	2.22	116.78	114.28
24	7	306	CHL	CHA-C1A-NA	2.22	131.48	126.40
29	9	301	0UR	C4-C3-C2	-2.22	118.17	120.08
33	i	101	LMG	C1-O6-C5	-2.22	109.33	113.69
31	D	410	8CT	C18-C19-C20	-2.22	118.93	123.47
25	B	602	CLA	O2D-CGD-CBD	2.22	115.21	111.27
28	g	304	NEX	C39-C29-C30	-2.22	119.81	122.92
29	7	301	0UR	C23-C24-C25	-2.22	108.63	113.64
28	S	617	NEX	C31-C32-C33	-2.22	120.18	126.42
24	3	317	CHL	O1D-CGD-CBD	-2.22	119.95	124.48
24	N	304	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
24	r	309	CHL	C4B-CHC-C1C	-2.22	121.08	126.34
24	R	608	CHL	C3C-C4C-NC	2.22	113.06	110.57
24	g	312	CHL	C4B-CHC-C1C	-2.22	121.08	126.34
24	Y	308	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
28	p	304	NEX	C31-C32-C33	-2.22	120.19	126.42
24	9	304	CHL	CHC-C4B-NB	-2.22	121.91	124.26
24	9	305	CHL	C3C-C4C-NC	2.21	113.06	110.57
24	Y	310	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
28	9	319	NEX	C31-C32-C33	-2.21	120.20	126.42
25	r	310	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
25	u	314	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	a	605	CLA	CHD-C1D-ND	-2.21	122.42	124.45
24	8	304	CHL	CHC-C4B-NB	-2.21	121.91	124.26
28	G	304	NEX	C31-C32-C33	-2.21	120.20	126.42
28	g	304	NEX	C31-C32-C33	-2.21	120.20	126.42
25	6	313	CLA	CMA-C3A-C2A	-2.21	110.94	116.10
29	8	301	0UR	C4-C5-C6	-2.21	116.31	123.22
25	4	313	CLA	C1-C2-C3	-2.21	122.22	126.04
24	1	310	CHL	C3C-C4C-NC	2.21	113.05	110.57
28	7	304	NEX	C31-C32-C33	-2.21	120.20	126.42
24	2	309	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
31	X	601	8CT	C40-C12-C13	-2.21	119.83	122.92
24	N	308	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
24	7	313	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
24	s	403	CHL	CHB-C4A-NA	2.21	127.57	124.51
24	y	311	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
24	S	613	CHL	C4B-CHC-C1C	-2.21	121.10	126.34
24	7	312	CHL	C4D-C3D-CAD	2.21	110.70	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	606	CHL	C4B-CHC-C1C	-2.21	121.10	126.34
35	a	606	PHO	C1-C2-C3	-2.21	122.22	126.04
28	4	303	NEX	C31-C32-C33	-2.21	120.22	126.42
24	p	313	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
24	6	311	CHL	C4D-C3D-CAD	2.21	110.70	108.10
24	7	305	CHL	C4D-C3D-CAD	2.21	110.70	108.10
33	D	411	LMG	O1-C1-C2	2.21	111.75	108.30
25	b	609	CLA	C3B-C4B-NB	-2.21	108.47	110.52
35	A	606	PHO	C1-C2-C3	-2.21	122.23	126.04
25	q	306	CLA	CHB-C4A-NA	2.21	127.56	124.51
30	d	408	LHG	O7-C7-O9	-2.21	118.37	123.70
25	1	313	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
25	5	308	CLA	CHD-C1D-ND	-2.21	122.43	124.45
25	A	603	CLA	CHB-C1B-NB	2.21	126.59	124.26
24	y	318	CHL	CHD-C1D-ND	-2.20	122.43	124.45
28	1	303	NEX	C31-C32-C33	-2.20	120.22	126.42
28	y	304	NEX	C31-C32-C33	-2.20	120.22	126.42
24	p	305	CHL	C4D-C3D-CAD	2.20	110.69	108.10
24	n	305	CHL	OMC-CMC-C2C	-2.20	120.70	125.69
25	3	316	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	B	613	CLA	CHB-C1B-NB	2.20	126.59	124.26
28	2	304	NEX	C31-C32-C33	-2.20	120.23	126.42
29	g	301	0UR	C15-C14-C13	-2.20	116.34	123.22
24	p	306	CHL	CHA-C1A-NA	2.20	131.44	126.40
25	p	314	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
24	3	317	CHL	C2A-C3A-C4A	-2.20	98.97	101.78
25	y	315	CLA	CHB-C4A-NA	2.20	127.56	124.51
24	3	311	CHL	C4D-C3D-CAD	2.20	110.69	108.10
33	W	201	LMG	O7-C10-O9	-2.20	118.38	123.70
26	n	302	0IE	C23-C16-C17	2.20	121.54	118.08
24	u	310	CHL	OMC-CMC-C2C	-2.20	120.71	125.69
25	N	313	CLA	CHD-C1D-ND	-2.20	122.43	124.45
29	7	301	0UR	C29-C30-C31	-2.20	109.24	111.74
25	A	607	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
25	y	307	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	b	613	CLA	CHB-C1B-NB	2.20	126.58	124.26
29	Y	301	0UR	C23-C24-C25	-2.20	108.68	113.64
24	G	306	CHL	C4B-CHC-C1C	-2.20	121.12	126.34
29	4	301	0UR	C33-C32-C31	-2.20	118.86	123.56
25	B	608	CLA	CHB-C1B-NB	2.20	126.58	124.26
24	p	312	CHL	C4B-CHC-C1C	-2.20	121.13	126.34
31	T	101	8CT	C27-C26-C25	-2.20	119.85	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
25	Y	313	CLA	CHB-C1B-NB	2.20	126.58	124.26
25	q	306	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	4	301	0UR	C24-C25-C26	-2.19	107.30	110.30
24	p	312	CHL	C4D-C3D-CAD	2.19	110.68	108.10
25	R	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
29	4	301	0UR	C34-C27-C26	2.19	118.42	114.36
28	N	303	NEX	C28-C29-C30	2.19	122.31	118.94
31	T	101	8CT	C24-C23-C21	-2.19	120.25	126.42
24	y	310	CHL	O2D-CGD-O1D	-2.19	119.55	123.84
24	Y	312	CHL	CMB-C2B-C1B	2.19	128.71	125.37
24	q	309	CHL	C4B-CHC-C1C	-2.19	121.14	126.34
25	b	602	CLA	O2D-CGD-CBD	2.19	115.16	111.27
25	R	604	CLA	CMA-C3A-C2A	-2.19	110.98	116.10
25	b	606	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
24	2	312	CHL	C4B-CHC-C1C	-2.19	121.14	126.34
23	E	201	HEM	C1B-NB-C4B	2.19	107.34	105.07
25	C	604	CLA	C1-C2-C3	-2.19	122.25	126.04
29	2	301	0UR	C21-C12-C11	-2.19	119.86	122.92
24	r	309	CHL	CHB-C4A-NA	2.19	127.54	124.51
31	C	613	8CT	C06-C07-C02	-2.19	110.17	114.08
24	n	308	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
24	y	313	CHL	CMB-C2B-C1B	2.19	128.70	125.37
29	5	301	0UR	C21-C12-C11	-2.19	119.86	122.92
24	p	312	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
24	3	304	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
24	1	305	CHL	OMC-CMC-C2C	-2.19	120.75	125.69
39	D	406	PL9	C37-C38-C39	-2.19	122.40	127.66
39	d	406	PL9	C37-C38-C39	-2.19	122.40	127.66
28	r	301	NEX	C28-C29-C30	2.18	122.29	118.94
24	G	311	CHL	CHC-C4B-NB	-2.18	121.94	124.26
25	n	313	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	b	607	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
25	a	603	CLA	CHB-C1B-NB	2.18	126.57	124.26
24	7	312	CHL	CHA-C1A-NA	2.18	131.39	126.40
31	C	613	8CT	C25-C24-C23	-2.18	116.41	123.22
24	u	306	CHL	C3C-C4C-NC	2.18	113.02	110.57
24	S	606	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
24	y	310	CHL	C4D-C3D-CAD	2.18	110.67	108.10
24	Y	319	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
25	B	609	CLA	CHC-C4B-NB	2.18	126.56	124.26
25	C	605	CLA	CHB-C1B-NB	2.18	126.56	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	310	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
28	6	303	NEX	C28-C29-C30	2.18	122.29	118.94
24	Y	319	CHL	C4A-NA-C1A	2.18	107.69	106.71
25	c	608	CLA	O2D-CGD-CBD	2.18	115.14	111.27
24	8	310	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
24	5	312	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
25	s	413	CLA	CHB-C1B-NB	2.18	126.56	124.26
28	6	303	NEX	C17-C1-C6	-2.18	108.52	110.47
25	B	606	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
31	X	601	8CT	C39-C16-C17	-2.18	119.87	122.92
31	x	601	8CT	C39-C16-C17	-2.18	119.87	122.92
24	S	605	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
24	Y	309	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
25	G	314	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	G	306	CHL	CHB-C4A-NA	2.18	127.52	124.51
25	b	605	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	s	414	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
24	Y	319	CHL	C4B-CHC-C1C	-2.18	121.18	126.34
24	q	309	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
33	w	201	LMG	O8-C28-O10	-2.18	118.10	123.59
24	S	608	CHL	C3C-C4C-NC	2.18	113.01	110.57
24	6	317	CHL	CHC-C4B-NB	-2.18	121.95	124.26
25	u	314	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
25	R	613	CLA	C3B-C4B-NB	-2.18	108.50	110.52
24	u	313	CHL	CHD-C1D-C2D	2.17	130.04	125.48
28	n	303	NEX	C28-C29-C30	2.17	122.28	118.94
24	4	310	CHL	C3C-C4C-NC	2.17	113.01	110.57
31	d	410	8CT	C14-C15-C16	-2.17	120.31	126.42
25	4	313	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
39	d	406	PL9	O1-C4-C3	-2.17	118.33	120.72
25	r	305	CLA	CHB-C1B-NB	2.17	126.56	124.26
24	G	318	CHL	C3C-C4C-NC	2.17	113.01	110.57
25	4	307	CLA	CMA-C3A-C2A	-2.17	111.03	116.10
24	5	309	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
26	u	303	0IE	C4-C5-C6	2.17	129.99	123.22
25	c	604	CLA	C1-C2-C3	-2.17	122.29	126.04
31	c	615	8CT	C13-C14-C15	-2.17	116.45	123.22
25	c	609	CLA	O1D-CGD-CBD	2.17	128.92	124.48
24	7	312	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
24	N	309	CHL	C4B-CHC-C1C	-2.17	121.19	126.34
31	B	617	8CT	C22-C21-C20	-2.17	119.89	122.92
24	q	311	CHL	C4B-CHC-C1C	-2.17	121.20	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	407	CHL	C4B-CHC-C1C	-2.17	121.20	126.34
25	C	609	CLA	O1D-CGD-CBD	2.17	128.92	124.48
31	t	101	8CT	C24-C23-C21	-2.17	120.33	126.42
25	Y	306	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
28	s	401	NEX	C17-C1-C6	-2.17	108.53	110.47
24	5	310	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
25	b	604	CLA	CHC-C4B-NB	2.17	126.55	124.26
24	4	311	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
24	p	318	CHL	C2A-C3A-C4A	-2.17	99.02	101.78
24	N	309	CHL	OMC-CMC-C2C	-2.17	120.79	125.69
24	R	607	CHL	C4B-CHC-C1C	-2.16	121.20	126.34
25	1	307	CLA	CMA-C3A-C2A	-2.16	111.05	116.10
24	y	305	CHL	CHA-C1A-NA	2.16	131.35	126.40
24	y	310	CHL	CHA-C1A-NA	2.16	131.35	126.40
24	q	308	CHL	C3D-C4D-CHA	-2.16	107.77	112.72
27	r	316	XAT	C20-C13-C12	2.16	121.49	118.08
25	B	609	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
24	2	306	CHL	C4B-CHC-C1C	-2.16	121.20	126.34
25	6	316	CLA	CHB-C1B-NB	2.16	126.55	124.26
24	Y	304	CHL	CHA-C1A-NA	2.16	131.35	126.40
25	B	607	CLA	O2D-CGD-CBD	2.16	115.11	111.27
25	b	616	CLA	CHC-C4B-NB	2.16	126.55	124.26
24	4	310	CHL	C4B-CHC-C1C	-2.16	121.21	126.34
24	q	304	CHL	CHB-C4A-NA	2.16	127.50	124.51
25	b	605	CLA	CHB-C1B-NB	2.16	126.55	124.26
25	6	313	CLA	CHD-C1D-ND	-2.16	122.47	124.45
25	9	313	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
25	8	312	CLA	C3B-C4B-NB	-2.16	108.51	110.52
24	7	311	CHL	O1D-CGD-CBD	-2.16	120.06	124.48
25	3	313	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	s	401	NEX	C28-C29-C30	2.16	122.26	118.94
25	a	607	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
25	8	305	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	N	309	CHL	CHA-C1A-NA	2.16	131.34	126.40
24	N	305	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
24	n	309	CHL	CHD-C1D-ND	-2.16	122.47	124.45
28	n	303	NEX	C17-C1-C6	-2.16	108.54	110.47
24	r	308	CHL	C4B-CHC-C1C	-2.16	121.22	126.34
24	g	311	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
25	B	605	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
39	D	406	PL9	C36-C34-C33	-2.16	116.75	121.12
25	c	603	CLA	CMB-C2B-C3B	2.16	131.81	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	615	8CT	C04-C03-C10	2.16	121.88	115.78
24	6	317	CHL	O1D-CGD-CBD	-2.16	120.07	124.48
24	r	303	CHL	C4B-CHC-C1C	-2.16	121.22	126.34
24	Y	311	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
25	2	314	CLA	CHB-C1B-NB	2.16	126.54	124.26
25	a	607	CLA	CHB-C1B-NB	2.16	126.54	124.26
25	r	311	CLA	CHB-C1B-NB	2.15	126.54	124.26
24	S	605	CHL	C3C-C4C-NC	2.15	112.99	110.57
28	3	318	NEX	C28-C29-C30	2.15	122.25	118.94
24	u	312	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
24	R	608	CHL	CHB-C4A-NA	2.15	127.49	124.51
24	9	311	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
27	r	316	XAT	C30-C31-C32	-2.15	116.50	123.22
24	7	305	CHL	C4B-CHC-C1C	-2.15	121.23	126.34
24	Y	309	CHL	C3D-C4D-CHA	-2.15	107.80	112.72
25	A	605	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	1	311	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
25	C	610	CLA	C1-C2-C3	-2.15	122.32	126.04
31	A	608	8CT	C05-C04-C03	2.15	113.79	110.48
31	a	608	8CT	C05-C04-C03	2.15	113.79	110.48
24	R	602	CHL	C4B-CHC-C1C	-2.15	121.24	126.34
24	p	305	CHL	C4B-CHC-C1C	-2.15	121.24	126.34
26	n	302	0IE	C5-C4-C3	2.15	129.59	127.00
24	p	318	CHL	CHC-C4B-NB	-2.15	121.98	124.26
25	s	412	CLA	CHB-C1B-NB	2.15	126.53	124.26
24	Y	317	CHL	CMA-C3A-C2A	-2.15	111.08	116.10
26	8	302	0IE	C4-C3-C2	-2.15	118.23	120.08
24	7	318	CHL	CHC-C4B-NB	-2.15	121.98	124.26
31	S	615	8CT	C11-C10-C03	-2.15	121.17	127.20
24	S	606	CHL	C4A-NA-C1A	2.15	107.67	106.71
25	C	603	CLA	CMB-C2B-C3B	2.15	131.79	126.59
24	1	310	CHL	C4B-CHC-C1C	-2.15	121.24	126.34
24	5	306	CHL	C4B-CHC-C1C	-2.15	121.24	126.34
25	c	606	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	g	314	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	Y	319	CHL	CHB-C4A-NA	2.15	127.48	124.51
28	3	318	NEX	C17-C1-C6	-2.15	108.55	110.47
28	N	303	NEX	C17-C1-C6	-2.15	108.55	110.47
24	7	311	CHL	CHC-C4B-NB	-2.15	121.98	124.26
24	s	406	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
31	b	617	8CT	C18-C19-C20	-2.15	119.08	123.47
25	u	308	CLA	O2A-CGA-O1A	-2.15	118.18	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	303	0IE	C23-C16-C17	2.15	121.46	118.08
25	b	610	CLA	C1-C2-C3	-2.15	122.33	126.04
24	q	311	CHL	C3C-C4C-NC	2.15	112.98	110.57
24	p	312	CHL	CHA-C1A-NA	2.14	131.31	126.40
25	B	610	CLA	C1-C2-C3	-2.14	122.33	126.04
25	S	612	CLA	CHB-C1B-NB	2.14	126.53	124.26
24	s	409	CHL	C3C-C4C-NC	2.14	112.97	110.57
25	p	307	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	8	308	CHL	C3D-C4D-CHA	-2.14	107.82	112.72
25	1	306	CLA	CHB-C1B-NB	2.14	126.53	124.26
24	Y	310	CHL	C1-O2A-CGA	2.14	122.06	116.44
25	g	314	CLA	C1-C2-C3	-2.14	122.34	126.04
25	B	605	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	6	313	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	B	607	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	p	315	CLA	C1-C2-C3	-2.14	122.34	126.04
25	2	307	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	b	608	CLA	CHB-C1B-NB	2.14	126.52	124.26
24	Y	309	CHL	CHB-C1B-C2B	-2.14	121.19	127.24
24	s	406	CHL	C3C-C4C-NC	2.14	112.97	110.57
24	s	407	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
33	d	401	LMG	O7-C10-O9	-2.14	118.53	123.70
25	c	616	CLA	CHB-C1B-NB	2.14	126.52	124.26
27	R	615	XAT	C30-C31-C32	-2.14	116.55	123.22
25	c	610	CLA	C1-C2-C3	-2.14	122.35	126.04
24	6	304	CHL	CHC-C4B-NB	-2.14	122.00	124.26
24	S	606	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
25	y	308	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	s	411	CLA	O1A-CGA-CBA	-2.14	112.88	126.89
25	4	313	CLA	CHD-C1D-ND	-2.13	122.49	124.45
25	c	603	CLA	CHB-C1B-NB	2.13	126.52	124.26
24	1	311	CHL	C3C-C4C-NC	2.13	112.97	110.57
27	R	615	XAT	C20-C13-C12	2.13	121.44	118.08
24	R	602	CHL	CHA-C1A-NA	2.13	131.28	126.40
24	r	303	CHL	CHA-C1A-NA	2.13	131.28	126.40
24	7	305	CHL	CHA-C1A-NA	2.13	131.28	126.40
24	Y	317	CHL	CHD-C1D-ND	-2.13	122.49	124.45
24	7	306	CHL	CHD-C1D-ND	-2.13	122.49	124.45
25	5	314	CLA	CHB-C1B-NB	2.13	126.52	124.26
24	p	305	CHL	CHA-C1A-NA	2.13	131.28	126.40
24	Y	310	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
25	B	604	CLA	C3B-C4B-NB	-2.13	108.54	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	407	CHL	C3C-C4C-NC	2.13	112.96	110.57
31	d	410	8CT	C18-C19-C20	-2.13	119.11	123.47
24	Y	319	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
31	v	401	8CT	C27-C26-C28	2.13	121.44	118.08
24	3	311	CHL	O2D-CGD-O1D	-2.13	119.67	123.84
29	Y	301	0UR	C24-C25-C26	-2.13	107.39	110.30
24	y	318	CHL	CMA-C3A-C2A	-2.13	111.12	116.10
24	7	313	CHL	C3C-C4C-NC	2.13	112.96	110.57
25	3	313	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	S	603	CLA	CHB-C1B-NB	2.13	126.51	124.26
24	s	414	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
25	7	307	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	S	611	CLA	CHB-C1B-NB	2.13	126.51	124.26
24	s	409	CHL	O2A-CGA-CBA	2.13	120.64	112.23
24	r	306	CHL	C4A-NA-C1A	2.13	107.66	106.71
24	7	318	CHL	C4A-NA-C1A	2.13	107.66	106.71
25	b	609	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
30	Y	318	LHG	C5-O7-C7	-2.13	112.55	117.79
24	N	311	CHL	C4B-CHC-C1C	-2.13	121.29	126.34
25	R	604	CLA	CHB-C1B-NB	2.13	126.51	124.26
29	1	301	0UR	C34-C27-C26	2.13	118.30	114.36
25	Y	313	CLA	CMB-C2B-C3B	2.13	131.74	126.59
25	n	313	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
31	C	613	8CT	C39-C16-C17	-2.13	119.94	122.92
24	8	310	CHL	C3C-C4C-NC	2.13	112.96	110.57
29	u	301	0UR	C9-C10-C11	-2.13	119.12	123.47
24	8	310	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
29	y	301	0UR	C23-C24-C25	-2.13	108.84	113.64
24	S	608	CHL	O2A-CGA-CBA	2.13	120.63	112.23
24	9	309	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
25	2	308	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	C	616	CLA	CHB-C1B-NB	2.12	126.51	124.26
24	4	305	CHL	OMC-CMC-C2C	-2.12	120.88	125.69
24	6	305	CHL	C3C-C4C-NC	2.12	112.95	110.57
24	y	310	CHL	C3D-C4D-CHA	-2.12	107.86	112.72
24	6	311	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
24	g	318	CHL	C3C-C4C-NC	2.12	112.95	110.57
31	V	401	8CT	C27-C26-C28	2.12	121.42	118.08
39	D	406	PL9	O1-C4-C3	-2.12	118.38	120.72
26	g	302	0IE	C23-C16-C17	2.12	121.42	118.08
24	r	302	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
25	n	307	CLA	CHD-C1D-ND	-2.12	122.50	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	601	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	C	603	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	a	605	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	n	309	CHL	C3D-C4D-CHA	-2.12	107.87	112.72
25	Y	307	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	8	308	CHL	C4B-CHC-C1C	-2.12	121.31	126.34
24	p	312	CHL	CHD-C1D-ND	-2.12	122.51	124.45
24	r	306	CHL	CHC-C4B-NB	-2.12	122.01	124.26
24	G	312	CHL	CHC-C4B-NB	-2.12	122.01	124.26
25	B	615	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	5	307	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	n	311	CHL	C4D-C3D-CAD	2.12	110.59	108.10
24	Y	305	CHL	CHD-C1D-ND	-2.12	122.51	124.45
25	B	605	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	q	305	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	b	607	CLA	O2D-CGD-CBD	2.12	115.03	111.27
25	G	308	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	g	308	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	A	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	g	313	CHL	CHD-C1D-C2D	2.11	129.92	125.48
24	n	309	CHL	C4B-CHC-C1C	-2.11	121.32	126.34
24	R	601	CHL	O1D-CGD-CBD	-2.11	120.16	124.48
25	c	601	CLA	C2D-C1D-ND	-2.11	108.55	110.10
26	3	302	0IE	C25-C24-C19	2.11	111.20	108.75
25	G	314	CLA	C1-C2-C3	-2.11	122.39	126.04
25	G	317	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	R	610	CLA	CHB-C1B-NB	2.11	126.49	124.26
24	8	304	CHL	CHB-C4A-NA	2.11	127.43	124.51
25	C	608	CLA	O2D-CGD-CBD	2.11	115.02	111.27
31	c	613	8CT	C39-C16-C17	-2.11	119.97	122.92
39	d	406	PL9	C36-C34-C33	-2.11	116.85	121.12
25	b	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
29	G	301	0UR	C22-C16-C17	2.11	121.40	118.08
24	R	602	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
25	9	313	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	b	613	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	D	404	CLA	C1-C2-C3	-2.11	122.39	126.04
24	5	311	CHL	O2A-CGA-CBA	2.11	120.57	112.23
25	b	615	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	G	308	CLA	CHD-C1D-ND	-2.11	122.52	124.45
24	q	308	CHL	CHA-C1A-NA	2.11	131.22	126.40
28	r	301	NEX	C17-C1-C6	-2.11	108.58	110.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	312	CHL	CAA-CBA-CGA	-2.11	107.09	113.25
24	q	311	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
24	n	311	CHL	C4B-CHC-C1C	-2.11	121.34	126.34
24	q	308	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
24	2	313	CHL	CHC-C4B-NB	-2.11	122.03	124.26
24	S	602	CHL	CHA-C1A-NA	2.11	131.22	126.40
24	5	312	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
25	5	317	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
23	f	201	HEM	C1B-NB-C4B	2.11	107.25	105.07
25	G	317	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
25	b	605	CLA	CHD-C1D-ND	-2.11	122.52	124.45
24	8	307	CHL	CHC-C4B-NB	-2.11	122.03	124.26
28	S	617	NEX	C40-C33-C34	-2.11	119.97	122.92
31	S	615	8CT	C15-C16-C17	2.10	122.17	118.94
24	S	606	CHL	CHC-C4B-NB	-2.10	122.03	124.26
25	r	304	CLA	CHC-C4B-NB	2.10	126.48	124.26
33	m	101	LMG	O7-C10-O9	-2.10	118.62	123.70
24	y	306	CHL	CHD-C1D-ND	-2.10	122.52	124.45
24	p	318	CHL	C3C-C4C-NC	2.10	112.93	110.57
24	s	407	CHL	C4A-NA-C1A	2.10	107.65	106.71
28	5	304	NEX	C40-C33-C34	-2.10	119.98	122.92
24	q	307	CHL	CHC-C4B-NB	-2.10	122.03	124.26
25	b	601	CLA	CHB-C1B-NB	2.10	126.48	124.26
25	7	315	CLA	C1-C2-C3	-2.10	122.41	126.04
25	3	314	CLA	C3B-C4B-NB	-2.10	108.56	110.52
25	S	604	CLA	CHC-C4B-NB	2.10	126.48	124.26
24	g	312	CHL	C3C-C4C-NC	2.10	112.93	110.57
28	N	303	NEX	C30-C31-C32	-2.10	116.66	123.22
29	q	301	0UR	C4-C5-C6	-2.10	116.66	123.22
28	2	304	NEX	C40-C33-C34	-2.10	119.98	122.92
24	2	311	CHL	O2A-CGA-CBA	2.10	120.53	112.23
24	Y	310	CHL	CHD-C1D-ND	-2.10	122.52	124.45
25	y	307	CLA	C1-C2-C3	-2.10	122.41	126.04
31	A	608	8CT	C40-C12-C13	-2.10	119.98	122.92
24	Y	309	CHL	CHD-C1D-ND	-2.10	122.52	124.45
25	G	314	CLA	CHD-C1D-ND	-2.10	122.52	124.45
24	4	311	CHL	C3C-C4C-NC	2.10	112.93	110.57
24	S	606	CHL	C3C-C4C-NC	2.10	112.92	110.57
25	7	317	CLA	CHB-C1B-NB	2.10	126.48	124.26
33	D	401	LMG	O7-C10-O9	-2.10	118.63	123.70
30	1	318	LHG	C26-C25-C24	2.10	120.73	113.19
32	a	609	SQD	O48-C23-C24	2.10	118.49	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	302	0IE	C25-C24-C19	2.10	111.18	108.75
25	a	607	CLA	O2D-CGD-CBD	2.10	115.00	111.27
24	r	303	CHL	OMC-CMC-C2C	-2.10	120.94	125.69
24	7	305	CHL	C3D-C4D-CHA	-2.10	107.93	112.72
25	B	604	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
24	s	407	CHL	CHC-C4B-NB	-2.10	122.04	124.26
28	9	319	NEX	C40-C33-C34	-2.10	119.99	122.92
25	3	314	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
29	G	301	0UR	C20-C7-C6	2.10	121.38	118.08
33	w	201	LMG	C7-O1-C1	-2.10	109.64	113.74
24	Y	304	CHL	C3D-C4D-CHA	-2.10	107.93	112.72
26	q	302	0IE	C4-C3-C2	-2.10	118.28	120.08
24	s	408	CHL	C4B-CHC-C1C	-2.09	121.37	126.34
25	a	604	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	n	305	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
25	A	607	CLA	O2D-CGD-CBD	2.09	114.99	111.27
25	y	317	CLA	CMB-C2B-C1B	-2.09	122.18	125.37
24	p	305	CHL	C3D-C4D-CHA	-2.09	107.93	112.72
30	4	318	LHG	C26-C25-C24	2.09	120.72	113.19
24	9	317	CHL	CHD-C1D-C2D	2.09	129.87	125.48
31	D	410	8CT	C25-C24-C23	-2.09	116.68	123.22
24	g	306	CHL	CHA-C1A-NA	2.09	131.19	126.40
24	p	313	CHL	C3C-C4C-NC	2.09	112.92	110.57
25	g	314	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	2	312	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
24	s	403	CHL	C4B-CHC-C1C	-2.09	121.37	126.34
26	u	302	0IE	C5-C4-C3	2.09	129.52	127.00
31	s	416	8CT	C15-C16-C17	2.09	122.15	118.94
25	C	607	CLA	CHC-C4B-NB	2.09	126.47	124.26
28	r	301	NEX	C30-C31-C32	-2.09	116.69	123.22
24	8	304	CHL	C4B-CHC-C1C	-2.09	121.38	126.34
25	b	604	CLA	C3B-C4B-NB	-2.09	108.58	110.52
24	9	312	CHL	CHD-C1D-C2D	2.09	129.87	125.48
28	6	303	NEX	C30-C31-C32	-2.09	116.69	123.22
37	c	619	DGD	O3D-C3D-C2D	-2.09	105.52	110.35
25	B	604	CLA	CHC-C4B-NB	2.09	126.47	124.26
28	g	304	NEX	C40-C33-C34	-2.09	120.00	122.92
24	R	607	CHL	CHA-C1A-NA	2.09	131.18	126.40
24	7	311	CHL	C3C-C4C-NC	2.09	112.92	110.57
29	u	301	0UR	C4-C5-C6	-2.09	116.69	123.22
32	A	609	SQD	O6-C1-C2	2.09	111.56	108.30
28	3	318	NEX	C30-C31-C32	-2.09	116.70	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	312	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
31	c	613	8CT	C37-C35-C30	-2.09	106.38	109.55
24	5	313	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
24	S	607	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
24	1	305	CHL	C4B-CHC-C1C	-2.09	121.39	126.34
25	N	306	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	y	315	CLA	CHC-C4B-NB	2.09	126.47	124.26
25	c	607	CLA	CHC-C4B-NB	2.09	126.47	124.26
25	r	313	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
25	g	317	CLA	CHD-C1D-ND	-2.09	122.54	124.45
29	g	301	0UR	C22-C16-C17	2.09	121.36	118.08
25	2	315	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	g	306	CHL	C4B-CHC-C1C	-2.09	121.39	126.34
25	q	306	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
28	s	401	NEX	C30-C31-C32	-2.09	116.71	123.22
29	u	301	0UR	C4-C3-C2	-2.09	118.29	120.08
24	4	312	CHL	O1D-CGD-CBD	-2.09	120.22	124.48
25	C	604	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	C	616	CLA	CHC-C4B-NB	2.09	126.47	124.26
33	W	201	LMG	C4-C3-C2	-2.09	107.18	110.82
25	R	613	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	c	604	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	6	314	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	s	413	CLA	CHC-C4B-NB	2.08	126.46	124.26
24	q	308	CHL	C4B-CHC-C1C	-2.08	121.40	126.34
32	b	618	SQD	C4-C3-C2	2.08	114.46	110.82
24	R	605	CHL	CHA-C1A-NA	2.08	131.17	126.40
25	Y	307	CLA	CHB-C1B-NB	2.08	126.46	124.26
28	p	304	NEX	C40-C33-C34	-2.08	120.01	122.92
24	7	309	CHL	CHD-C1D-C2D	2.08	129.85	125.48
24	R	606	CHL	C4A-NA-C1A	2.08	107.64	106.71
25	R	611	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	4	306	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	c	610	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	C	610	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
24	1	304	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
24	N	309	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
24	8	308	CHL	CHA-C1A-NA	2.08	131.16	126.40
25	8	306	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	R	608	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
24	4	305	CHL	C4B-CHC-C1C	-2.08	121.40	126.34
25	B	603	CLA	CHB-C1B-NB	2.08	126.46	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	405	CLA	CHC-C4B-NB	2.08	126.46	124.26
25	c	616	CLA	O2D-CGD-CBD	2.08	114.96	111.27
24	7	318	CHL	C2A-C3A-C4A	-2.08	99.13	101.78
28	n	303	NEX	C30-C31-C32	-2.08	116.73	123.22
25	C	610	CLA	CHD-C1D-ND	-2.08	122.55	124.45
24	r	306	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
24	S	613	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
25	B	602	CLA	CMB-C2B-C1B	-2.08	122.21	125.37
25	r	314	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	r	316	XAT	C38-C25-C24	2.08	116.61	114.28
24	2	312	CHL	C4D-C3D-CAD	2.08	110.54	108.10
28	r	317	NEX	C40-C33-C34	-2.08	120.02	122.92
25	b	603	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
24	y	312	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
25	Y	316	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
25	B	613	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
25	b	604	CLA	CAA-CBA-CGA	-2.07	107.19	113.25
24	4	311	CHL	C4B-CHC-C1C	-2.07	121.42	126.34
25	A	605	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	y	305	CHL	C3D-C4D-CHA	-2.07	107.98	112.72
25	2	317	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	G	313	CHL	CHD-C1D-C2D	2.07	129.83	125.48
30	a	612	LHG	C26-C25-C24	2.07	120.64	113.19
25	r	314	CLA	C3B-C4B-NB	-2.07	108.59	110.52
24	q	308	CHL	O1D-CGD-CBD	-2.07	120.24	124.48
25	B	608	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	N	311	CHL	C4D-C3D-CAD	2.07	110.54	108.10
24	N	312	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
24	q	309	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
28	R	616	NEX	C40-C33-C34	-2.07	120.02	122.92
26	7	302	0IE	C14-C15-C16	2.07	130.27	127.31
25	C	616	CLA	O2D-CGD-CBD	2.07	114.95	111.27
24	y	310	CHL	CHD-C1D-ND	-2.07	122.55	124.45
25	C	605	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	3	315	CLA	CHB-C1B-NB	2.07	126.45	124.26
24	g	305	CHL	C3C-C4C-NC	2.07	112.89	110.57
24	Y	308	CHL	CHC-C4B-NB	-2.07	122.07	124.26
25	4	306	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
30	A	612	LHG	C26-C25-C24	2.07	120.63	113.19
26	p	302	0IE	C14-C15-C16	2.07	130.26	127.31
28	7	304	NEX	C40-C33-C34	-2.07	120.03	122.92
24	g	306	CHL	C3D-C4D-CHA	-2.07	107.99	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	313	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
25	n	307	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
24	5	305	CHL	C3C-C4C-NC	2.07	112.89	110.57
25	g	317	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
24	1	311	CHL	C4B-CHC-C1C	-2.07	121.43	126.34
24	1	312	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
24	Y	312	CHL	C3C-C4C-NC	2.07	112.89	110.57
24	N	305	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
36	a	611	BCT	O3-C-O1	-2.07	114.19	119.55
24	r	308	CHL	CHA-C1A-NA	2.07	131.13	126.40
24	Y	317	CHL	C2A-C3A-C4A	-2.07	99.15	101.78
31	C	615	8CT	C13-C14-C15	-2.07	116.77	123.22
24	S	607	CHL	C4B-CHC-C1C	-2.07	121.44	126.34
24	q	304	CHL	C4B-CHC-C1C	-2.07	121.44	126.34
24	7	318	CHL	C3C-C4C-NC	2.07	112.89	110.57
25	B	603	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
25	A	610	CLA	CHD-C1D-ND	-2.06	122.56	124.45
24	3	305	CHL	C3C-C4C-NC	2.06	112.89	110.57
24	s	403	CHL	CHA-C1A-NA	2.06	131.12	126.40
25	S	603	CLA	CHC-C4B-NB	2.06	126.44	124.26
25	q	306	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
25	s	404	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	Y	312	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
24	N	317	CHL	C2A-C1A-CHA	-2.06	120.25	123.85
24	R	605	CHL	CAA-C2A-C3A	-2.06	111.29	116.10
24	8	307	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
25	C	602	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	c	616	CLA	CHC-C4B-NB	2.06	126.44	124.26
26	G	303	0IE	C23-C16-C17	2.06	121.32	118.08
24	8	309	CHL	CHA-C1A-NA	2.06	131.11	126.40
24	6	309	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
24	4	304	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
25	G	317	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	A	607	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	5	315	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	G	313	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
24	u	318	CHL	CHD-C1D-C2D	2.06	129.79	125.48
29	3	301	0UR	C10-C9-C8	-2.06	119.26	123.47
24	R	608	CHL	O2A-CGA-CBA	2.06	120.64	114.03
25	C	601	CLA	C1-C2-C3	-2.06	122.49	126.04
25	r	312	CLA	CHB-C1B-NB	2.06	126.43	124.26
24	7	305	CHL	CHC-C1C-C2C	-2.06	118.66	126.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	311	CHL	C3C-C4C-NC	2.06	112.88	110.57
28	u	304	NEX	C40-C33-C34	-2.06	120.04	122.92
24	8	308	CHL	OMC-CMC-C2C	-2.06	121.04	125.69
24	g	312	CHL	CHC-C4B-NB	-2.05	122.08	124.26
24	r	308	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
24	G	305	CHL	CHC-C4B-NB	-2.05	122.08	124.26
25	d	405	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	b	602	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
24	Y	309	CHL	O2A-CGA-CBA	2.05	120.34	112.23
24	q	311	CHL	CHB-C4A-NA	2.05	127.35	124.51
24	s	408	CHL	O2D-CGD-O1D	-2.05	119.83	123.84
25	c	610	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
24	q	310	CHL	CHA-C1A-NA	2.05	131.09	126.40
25	c	609	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	3	309	CHL	CHC-C4B-NB	-2.05	122.09	124.26
25	5	317	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	1	313	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	y	317	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	N	307	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	y	306	CHL	CHA-C1A-NA	2.05	131.09	126.40
24	N	309	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
24	y	318	CHL	C2A-C3A-C4A	-2.05	99.17	101.78
25	9	314	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	B	606	CLA	CHC-C4B-NB	2.05	126.43	124.26
25	u	308	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	B	609	CLA	C1-C2-C3	-2.05	122.50	126.04
24	y	310	CHL	O2A-CGA-CBA	2.05	120.33	112.23
25	y	314	CLA	CMB-C2B-C3B	2.05	131.55	126.59
24	3	309	CHL	OMC-CMC-C2C	-2.05	121.06	125.69
32	B	618	SQD	C4-C3-C2	2.05	114.40	110.82
24	S	602	CHL	C4B-CHC-C1C	-2.05	121.48	126.34
24	R	607	CHL	C3D-C4D-CHA	-2.05	108.04	112.72
35	d	403	PHO	O2A-CGA-O1A	-2.05	118.42	123.59
31	d	410	8CT	C25-C24-C23	-2.05	116.83	123.22
25	r	311	CLA	CMB-C2B-C3B	2.05	131.55	126.59
25	6	315	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	u	315	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	R	605	CHL	C3D-C4D-CHA	-2.05	108.04	112.72
24	4	305	CHL	CHC-C4B-NB	-2.05	122.09	124.26
25	g	308	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	c	609	CLA	C1-C2-C3	-2.05	122.50	126.04
29	Y	301	0UR	C22-C16-C17	2.05	121.30	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	311	CHL	O2D-CGD-O1D	-2.05	119.84	123.84
24	g	312	CHL	O2D-CGD-O1D	-2.04	119.84	123.84
24	r	309	CHL	O1D-CGD-CBD	-2.04	120.30	124.48
25	R	612	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
24	y	306	CHL	C6-C5-C3	-2.04	108.09	113.45
28	1	303	NEX	C40-C33-C34	-2.04	120.06	122.92
25	1	306	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
24	p	305	CHL	CHC-C1C-C2C	-2.04	118.70	126.11
24	Y	311	CHL	CHA-C1A-NA	2.04	131.07	126.40
24	5	312	CHL	C4D-C3D-CAD	2.04	110.50	108.10
24	n	312	CHL	O1D-CGD-CBD	-2.04	120.30	124.48
24	8	307	CHL	C3C-C4C-NC	2.04	112.86	110.57
24	n	312	CHL	C3C-C4C-NC	2.04	112.86	110.57
25	R	609	CLA	C1-C2-C3	-2.04	122.51	126.04
25	c	601	CLA	CMB-C2B-C3B	2.04	131.53	126.59
25	p	317	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	s	404	CLA	CHC-C4B-NB	2.04	126.42	124.26
25	6	315	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
25	b	608	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
31	C	614	8CT	C39-C16-C17	-2.04	120.06	122.92
23	E	201	HEM	C4C-NC-C1C	2.04	107.35	105.35
26	g	303	0IE	C23-C16-C17	2.04	121.29	118.08
25	8	306	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
25	C	601	CLA	CMB-C2B-C3B	2.04	131.53	126.59
25	8	314	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	b	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	N	306	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	9	301	0UR	C4-C5-C6	-2.04	116.85	123.22
24	3	312	CHL	CHD-C1D-C2D	2.04	129.76	125.48
33	d	411	LMG	O1-C7-C8	-2.04	105.98	110.90
36	A	611	BCT	O3-C-O1	-2.04	114.26	119.55
24	p	306	CHL	CHC-C1C-C2C	-2.04	118.72	126.11
28	4	303	NEX	C40-C33-C34	-2.04	120.07	122.92
25	3	316	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	b	607	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	y	312	CHL	CHB-C4A-NA	2.04	127.33	124.51
24	y	312	CHL	CHA-C1A-NA	2.04	131.06	126.40
24	g	309	CHL	C2A-C1A-CHA	-2.04	120.30	123.86
24	g	310	CHL	O2A-CGA-CBA	2.04	120.28	112.23
25	6	316	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	A	608	8CT	C39-C16-C17	-2.04	120.07	122.92
25	y	308	CLA	CHB-C1B-NB	2.04	126.41	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	318	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
24	N	317	CHL	CHD-C1D-C2D	2.04	129.75	125.48
25	R	603	CLA	CHC-C4B-NB	2.04	126.41	124.26
24	g	318	CHL	OMC-CMC-C2C	-2.03	121.09	125.69
24	r	309	CHL	O2A-CGA-CBA	2.03	120.57	114.03
25	3	314	CLA	CHB-C1B-NB	2.03	126.41	124.26
24	7	306	CHL	C3D-C4D-CHA	-2.03	108.07	112.72
24	7	310	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
25	D	405	CLA	C1-C2-C3	-2.03	122.53	126.04
24	G	305	CHL	C3C-C4C-NC	2.03	112.85	110.57
26	9	303	0IE	C15-C14-C13	2.03	129.56	123.22
25	a	610	CLA	CHD-C1D-ND	-2.03	122.58	124.45
24	g	313	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
39	D	406	PL9	C12-C13-C14	-2.03	122.76	127.66
25	C	603	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	c	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	2	305	CHL	C3C-C4C-NC	2.03	112.85	110.57
24	q	308	CHL	C4D-C3D-CAD	2.03	110.49	108.10
24	s	408	CHL	O2A-CGA-CBA	2.03	120.56	114.03
25	b	603	CLA	CHB-C1B-NB	2.03	126.41	124.26
24	3	310	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
24	n	309	CHL	CHC-C1C-C2C	-2.03	118.74	126.11
25	C	609	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	8	308	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
25	3	315	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
24	N	312	CHL	C3C-C4C-NC	2.03	112.85	110.57
25	b	609	CLA	C1-C2-C3	-2.03	122.53	126.04
26	5	303	0IE	C23-C16-C17	2.03	121.28	118.08
25	B	608	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
25	a	607	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	c	603	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	n	311	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
25	g	317	CLA	CHB-C1B-NB	2.03	126.41	124.26
25	n	306	CLA	CHB-C1B-NB	2.03	126.41	124.26
24	6	305	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
24	G	310	CHL	O2A-CGA-CBA	2.03	120.25	112.23
25	Y	307	CLA	CMB-C2B-C3B	2.03	131.50	126.59
25	s	405	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	N	312	CHL	OMC-CMC-C2C	-2.03	121.10	125.69
25	q	306	CLA	CHB-C1B-NB	2.03	126.40	124.26
24	G	312	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
24	5	305	CHL	OMC-CMC-C2C	-2.03	121.10	125.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	317	CHL	C2A-C1A-CHA	-2.03	120.31	123.85
37	C	620	DGD	C3D-C4D-C5D	2.03	113.86	110.24
24	y	311	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
24	Y	304	CHL	C4D-C3D-CAD	2.03	110.48	108.10
24	y	305	CHL	C4D-C3D-CAD	2.03	110.48	108.10
31	c	614	8CT	C10-C03-C02	-2.03	116.55	121.46
24	9	308	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
24	n	309	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
33	W	201	LMG	O8-C28-O10	-2.03	118.48	123.59
28	y	304	NEX	C40-C33-C34	-2.03	120.08	122.92
29	y	301	0UR	C22-C16-C17	2.03	121.27	118.08
24	y	313	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
31	c	614	8CT	C39-C16-C17	-2.03	120.09	122.92
30	5	319	LHG	C26-C25-C24	2.02	120.47	113.19
24	p	310	CHL	O1D-CGD-CBD	-2.02	120.34	124.48
25	b	609	CLA	CHC-C4B-NB	2.02	126.40	124.26
24	7	306	CHL	CHC-C1C-C2C	-2.02	118.77	126.11
29	y	301	0UR	C14-C15-C16	-2.02	124.42	127.31
25	g	307	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
24	y	309	CHL	C3C-C4C-NC	2.02	112.84	110.57
31	V	401	8CT	C13-C14-C15	-2.02	116.91	123.22
25	D	404	CLA	O2D-CGD-CBD	2.02	114.86	111.27
24	p	306	CHL	C3D-C4D-CHA	-2.02	108.10	112.72
25	5	308	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	R	604	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	N	313	CLA	CHB-C1B-NB	2.02	126.40	124.26
25	s	411	CLA	CHC-C4B-NB	2.02	126.40	124.26
24	1	305	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
25	S	611	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
25	c	601	CLA	C1-C2-C3	-2.02	122.55	126.04
29	9	301	0UR	C29-C30-C31	-2.02	109.44	111.74
24	p	309	CHL	CHD-C1D-C2D	2.02	129.72	125.48
28	G	304	NEX	C40-C33-C34	-2.02	120.09	122.92
24	3	311	CHL	C4B-CHC-C1C	-2.02	121.55	126.34
24	q	304	CHL	C3D-C4D-CHA	-2.02	108.10	112.72
25	D	405	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	s	417	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	Y	305	CHL	CHA-C1A-NA	2.02	131.02	126.40
25	C	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
27	R	615	XAT	O4-C5-C6	-2.02	57.29	58.96
29	3	301	0UR	C34-C27-C26	2.02	118.09	114.36
25	A	610	CLA	CHB-C1B-NB	2.02	126.39	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	301	0UR	C20-C7-C6	2.02	121.26	118.08
30	5	319	LHG	C5-O7-C7	-2.02	112.82	117.79
29	6	301	0UR	C4-C5-C6	-2.02	116.92	123.22
25	3	316	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
25	S	612	CLA	CHC-C4B-NB	2.02	126.39	124.26
25	c	602	CLA	CHB-C1B-NB	2.02	126.39	124.26
39	d	406	PL9	C12-C13-C14	-2.02	122.80	127.66
30	a	601	LHG	C26-C25-C24	2.02	120.44	113.19
25	C	609	CLA	C1-C2-C3	-2.02	122.55	126.04
25	s	412	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
26	u	302	0IE	C23-C16-C17	2.02	121.25	118.08
32	a	609	SQD	C4-C3-C2	2.02	114.34	110.82
29	g	301	0UR	C23-C24-C25	-2.02	109.09	113.64
24	7	312	CHL	CHC-C1C-C2C	-2.02	118.80	126.11
25	2	308	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	9	306	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	Y	306	CLA	C1-C2-C3	-2.02	122.56	126.04
30	p	319	LHG	C26-C25-C24	2.01	120.43	113.19
25	u	315	CLA	CHB-C1B-NB	2.01	126.39	124.26
25	r	313	CLA	CHC-C4B-NB	2.01	126.39	124.26
24	Y	305	CHL	C6-C5-C3	-2.01	108.17	113.45
30	2	319	LHG	C26-C25-C24	2.01	120.43	113.19
24	n	317	CHL	CHD-C1D-C2D	2.01	129.71	125.48
24	4	305	CHL	O1D-CGD-CBD	-2.01	120.36	124.48
25	n	306	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	p	318	CHL	C4A-NA-C1A	2.01	107.61	106.71
25	C	610	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
37	c	618	DGD	O6D-C5D-C4D	-2.01	106.04	109.69
25	2	314	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	4	313	CLA	CHB-C1B-NB	2.01	126.39	124.26
25	c	610	CLA	CHB-C1B-NB	2.01	126.39	124.26
24	6	311	CHL	C3D-C4D-CHA	-2.01	108.12	112.72
29	6	301	0UR	C15-C14-C13	-2.01	116.94	123.22
25	9	316	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	1	316	CLA	CHB-C1B-NB	2.01	126.39	124.26
25	b	603	CLA	CHC-C4B-NB	2.01	126.39	124.26
31	v	401	8CT	C13-C14-C15	-2.01	116.94	123.22
25	d	404	CLA	O2D-CGD-CBD	2.01	114.84	111.27
25	9	316	CLA	CHB-C1B-NB	2.01	126.39	124.26
25	4	307	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	y	301	0UR	C28-C19-C18	-2.01	110.16	112.70
24	q	310	CHL	C3D-C4D-CHA	-2.01	108.12	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	311	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
24	2	312	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
24	S	607	CHL	O2A-CGA-CBA	2.01	120.48	114.03
25	6	306	CLA	CHB-C1B-NB	2.01	126.38	124.26
31	D	410	8CT	C14-C15-C16	-2.01	120.77	126.42
24	p	312	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
31	C	614	8CT	C10-C03-C02	-2.01	116.60	121.46
25	S	610	CLA	CHC-C4B-NB	2.01	126.38	124.26
25	B	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	G	307	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
25	S	616	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	y	307	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	6	309	CHL	C3C-C4C-NC	2.01	112.82	110.57
24	1	305	CHL	O2A-CGA-CBA	2.01	120.48	114.03
25	C	612	CLA	C1-C2-C3	-2.01	122.57	126.04
25	c	602	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
24	G	306	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
25	c	601	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
24	S	608	CHL	CHC-C1C-C2C	-2.01	118.83	126.11
24	1	305	CHL	CHA-C1A-NA	2.01	130.99	126.40
32	D	409	SQD	C4-C3-C2	2.01	114.32	110.82
25	5	308	CLA	CHB-C1B-NB	2.01	126.38	124.26
26	y	303	0IE	C17-C16-C15	2.01	122.02	118.94
24	y	311	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
24	y	311	CHL	CHA-C1A-NA	2.01	130.99	126.40
24	4	309	CHL	OMC-CMC-C2C	-2.00	121.15	125.69
31	a	608	8CT	C39-C16-C17	-2.00	120.11	122.92
24	g	305	CHL	CHC-C4B-NB	-2.00	122.14	124.26
24	y	309	CHL	CHC-C4B-NB	-2.00	122.14	124.26
24	4	312	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
25	b	612	CLA	CMB-C2B-C3B	2.00	131.44	126.59
24	7	312	CHL	C3D-C4D-CHA	-2.00	108.14	112.72
24	S	608	CHL	CHA-C1A-NA	2.00	130.99	126.40
31	D	410	8CT	C27-C26-C28	2.00	121.23	118.08
25	c	604	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	7	315	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	p	306	CHL	CHD-C1D-ND	-2.00	122.61	124.45
24	Y	311	CHL	CHB-C4A-NA	2.00	127.28	124.51
25	C	608	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
24	y	310	CHL	CHB-C1B-C2B	-2.00	121.58	127.24
25	8	312	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	c	608	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	305	CHL	CHC-C4B-NB	-2.00	122.14	124.26
24	y	311	CHL	C3D-C4D-CHA	-2.00	108.14	112.72
24	g	318	CHL	C2A-C3A-C4A	-2.00	99.23	101.78
25	B	601	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	c	609	CLA	CHD-C1D-ND	-2.00	122.61	124.45
24	8	309	CHL	C3D-C4D-CHA	-2.00	108.14	112.72
24	3	304	CHL	C3C-C4C-NC	2.00	112.81	110.57
25	N	315	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
25	y	308	CLA	CMB-C2B-C3B	2.00	131.43	126.59
24	n	312	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
28	n	303	NEX	C40-C33-C34	-2.00	120.12	122.92
24	G	309	CHL	CHD-C1D-C2D	2.00	129.68	125.48
25	4	316	CLA	CHD-C1D-ND	-2.00	122.62	124.45

There are no chirality outliers.

All (4494) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	R	601	CHL	C3C-C2C-CMC-OMC
24	R	607	CHL	C3C-C2C-CMC-OMC
24	1	305	CHL	CHA-CBD-CGD-O1D
24	1	305	CHL	CHA-CBD-CGD-O2D
24	1	317	CHL	CHA-CBD-CGD-O1D
24	1	317	CHL	CHA-CBD-CGD-O2D
24	1	317	CHL	CAD-CBD-CGD-O1D
24	2	305	CHL	C3C-C2C-CMC-OMC
24	2	306	CHL	C3C-C2C-CMC-OMC
24	2	306	CHL	CHA-CBD-CGD-O1D
24	2	306	CHL	CHA-CBD-CGD-O2D
24	2	312	CHL	C3C-C2C-CMC-OMC
24	2	312	CHL	CBD-CGD-O2D-CED
24	2	318	CHL	CHA-CBD-CGD-O1D
24	2	318	CHL	CHA-CBD-CGD-O2D
24	2	318	CHL	CAD-CBD-CGD-O1D
24	3	304	CHL	C1A-C2A-CAA-CBA
24	3	304	CHL	C3A-C2A-CAA-CBA
24	3	305	CHL	C2B-C3B-CAB-CBB
24	3	305	CHL	C4B-C3B-CAB-CBB
24	3	305	CHL	C1C-C2C-CMC-OMC
24	3	305	CHL	C3C-C2C-CMC-OMC
24	3	305	CHL	CHA-CBD-CGD-O1D
24	3	305	CHL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	S	601	CHL	C2B-C3B-CAB-CBB
24	S	601	CHL	C4B-C3B-CAB-CBB
24	S	601	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C3C-C2C-CMC-OMC
24	S	602	CHL	C3C-C2C-CMC-OMC
24	S	602	CHL	CHA-CBD-CGD-O1D
24	S	602	CHL	CHA-CBD-CGD-O2D
24	S	607	CHL	C1A-C2A-CAA-CBA
24	S	607	CHL	C3A-C2A-CAA-CBA
24	S	608	CHL	C3C-C2C-CMC-OMC
24	S	613	CHL	C3C-C2C-CMC-OMC
24	G	305	CHL	C1A-C2A-CAA-CBA
24	G	305	CHL	C3A-C2A-CAA-CBA
24	G	306	CHL	C3C-C2C-CMC-OMC
24	G	306	CHL	CHA-CBD-CGD-O1D
24	G	306	CHL	CHA-CBD-CGD-O2D
24	G	306	CHL	C6-C7-C8-C9
24	G	311	CHL	CBD-CGD-O2D-CED
24	G	312	CHL	C2A-CAA-CBA-CGA
24	G	312	CHL	CBD-CGD-O2D-CED
24	G	318	CHL	C3C-C2C-CMC-OMC
24	G	318	CHL	CHA-CBD-CGD-O1D
24	G	318	CHL	CHA-CBD-CGD-O2D
24	G	318	CHL	CAD-CBD-CGD-O1D
24	G	318	CHL	CAD-CBD-CGD-O2D
24	9	304	CHL	C3C-C2C-CMC-OMC
24	9	305	CHL	C1C-C2C-CMC-OMC
24	9	305	CHL	C3C-C2C-CMC-OMC
24	9	305	CHL	CHA-CBD-CGD-O1D
24	9	305	CHL	CHA-CBD-CGD-O2D
24	9	310	CHL	C1A-C2A-CAA-CBA
24	9	310	CHL	C3A-C2A-CAA-CBA
24	9	311	CHL	C1A-C2A-CAA-CBA
24	9	312	CHL	CBD-CGD-O2D-CED
24	9	317	CHL	CHA-CBD-CGD-O1D
24	9	317	CHL	CHA-CBD-CGD-O2D
24	9	317	CHL	CAD-CBD-CGD-O1D
24	N	305	CHL	C3C-C2C-CMC-OMC
24	N	305	CHL	CHA-CBD-CGD-O2D
24	N	309	CHL	C3C-C2C-CMC-OMC
24	N	311	CHL	CBD-CGD-O2D-CED
24	N	312	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Y	305	CHL	CHA-CBD-CGD-O1D
24	Y	305	CHL	CHA-CBD-CGD-O2D
24	Y	308	CHL	C3C-C2C-CMC-OMC
24	Y	310	CHL	C3C-C2C-CMC-OMC
24	Y	311	CHL	C1C-C2C-CMC-OMC
24	Y	311	CHL	C3C-C2C-CMC-OMC
24	Y	312	CHL	C1C-C2C-CMC-OMC
24	Y	312	CHL	C3C-C2C-CMC-OMC
24	Y	312	CHL	C6-C7-C8-C9
24	Y	317	CHL	C3C-C2C-CMC-OMC
24	8	303	CHL	C1A-C2A-CAA-CBA
24	8	303	CHL	C3A-C2A-CAA-CBA
24	8	303	CHL	C2-C3-C5-C6
24	8	303	CHL	C4-C3-C5-C6
24	8	304	CHL	C3C-C2C-CMC-OMC
24	8	304	CHL	CHA-CBD-CGD-O1D
24	8	304	CHL	CHA-CBD-CGD-O2D
24	8	310	CHL	C3C-C2C-CMC-OMC
24	4	305	CHL	CHA-CBD-CGD-O1D
24	4	305	CHL	CHA-CBD-CGD-O2D
24	4	312	CHL	C3C-C2C-CMC-OMC
24	4	317	CHL	CHA-CBD-CGD-O1D
24	4	317	CHL	CHA-CBD-CGD-O2D
24	4	317	CHL	CAD-CBD-CGD-O1D
24	5	305	CHL	C3C-C2C-CMC-OMC
24	5	306	CHL	C3C-C2C-CMC-OMC
24	5	306	CHL	CHA-CBD-CGD-O1D
24	5	306	CHL	CHA-CBD-CGD-O2D
24	5	312	CHL	C3C-C2C-CMC-OMC
24	5	312	CHL	CBD-CGD-O2D-CED
24	5	318	CHL	CHA-CBD-CGD-O1D
24	5	318	CHL	CHA-CBD-CGD-O2D
24	5	318	CHL	CAD-CBD-CGD-O1D
24	6	304	CHL	C1A-C2A-CAA-CBA
24	6	304	CHL	C3A-C2A-CAA-CBA
24	6	304	CHL	C3C-C2C-CMC-OMC
24	6	305	CHL	C2B-C3B-CAB-CBB
24	6	305	CHL	C4B-C3B-CAB-CBB
24	6	305	CHL	C1C-C2C-CMC-OMC
24	6	305	CHL	C3C-C2C-CMC-OMC
24	6	305	CHL	CHA-CBD-CGD-O1D
24	6	305	CHL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	g	305	CHL	C1A-C2A-CAA-CBA
24	g	305	CHL	C3A-C2A-CAA-CBA
24	g	306	CHL	C3C-C2C-CMC-OMC
24	g	306	CHL	CHA-CBD-CGD-O1D
24	g	306	CHL	CHA-CBD-CGD-O2D
24	g	312	CHL	C2A-CAA-CBA-CGA
24	g	312	CHL	CBD-CGD-O2D-CED
24	g	313	CHL	CHA-CBD-CGD-O1D
24	g	318	CHL	C3C-C2C-CMC-OMC
24	g	318	CHL	CHA-CBD-CGD-O1D
24	g	318	CHL	CHA-CBD-CGD-O2D
24	g	318	CHL	CAD-CBD-CGD-O1D
24	g	318	CHL	CAD-CBD-CGD-O2D
24	u	306	CHL	C1C-C2C-CMC-OMC
24	u	306	CHL	C3C-C2C-CMC-OMC
24	u	306	CHL	CHA-CBD-CGD-O1D
24	u	306	CHL	CHA-CBD-CGD-O2D
24	u	310	CHL	C3C-C2C-CMC-OMC
24	u	318	CHL	CHA-CBD-CGD-O1D
24	u	318	CHL	CHA-CBD-CGD-O2D
24	u	318	CHL	CAD-CBD-CGD-O1D
24	n	305	CHL	C3C-C2C-CMC-OMC
24	n	311	CHL	C2A-CAA-CBA-CGA
24	n	311	CHL	CBD-CGD-O2D-CED
24	n	312	CHL	C3C-C2C-CMC-OMC
24	y	305	CHL	C11-C12-C13-C14
24	y	306	CHL	CHA-CBD-CGD-O1D
24	y	306	CHL	CHA-CBD-CGD-O2D
24	y	309	CHL	C3C-C2C-CMC-OMC
24	y	311	CHL	C3C-C2C-CMC-OMC
24	y	312	CHL	C3C-C2C-CMC-OMC
24	y	313	CHL	C1C-C2C-CMC-OMC
24	y	313	CHL	C3C-C2C-CMC-OMC
24	y	313	CHL	C6-C7-C8-C9
24	y	318	CHL	C3C-C2C-CMC-OMC
24	p	306	CHL	C1C-C2C-CMC-OMC
24	p	306	CHL	CHA-CBD-CGD-O1D
24	p	306	CHL	CHA-CBD-CGD-O2D
24	p	310	CHL	C1C-C2C-CMC-OMC
24	p	310	CHL	C3C-C2C-CMC-OMC
24	p	312	CHL	C1C-C2C-CMC-OMC
24	p	312	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	p	312	CHL	CBD-CGD-O2D-CED
24	q	303	CHL	C1A-C2A-CAA-CBA
24	q	303	CHL	C3A-C2A-CAA-CBA
24	q	303	CHL	C2-C3-C5-C6
24	q	303	CHL	C4-C3-C5-C6
24	q	304	CHL	C3C-C2C-CMC-OMC
24	q	304	CHL	CHA-CBD-CGD-O1D
24	q	304	CHL	CHA-CBD-CGD-O2D
24	q	311	CHL	C3C-C2C-CMC-OMC
24	s	402	CHL	C2B-C3B-CAB-CBB
24	s	402	CHL	C4B-C3B-CAB-CBB
24	s	402	CHL	C1C-C2C-CMC-OMC
24	s	402	CHL	C3C-C2C-CMC-OMC
24	s	403	CHL	C3C-C2C-CMC-OMC
24	s	403	CHL	CHA-CBD-CGD-O1D
24	s	403	CHL	CHA-CBD-CGD-O2D
24	s	408	CHL	C1A-C2A-CAA-CBA
24	s	408	CHL	C3A-C2A-CAA-CBA
24	s	409	CHL	C3C-C2C-CMC-OMC
24	s	414	CHL	C3C-C2C-CMC-OMC
24	r	302	CHL	C3C-C2C-CMC-OMC
24	r	306	CHL	C3C-C2C-CMC-OMC
24	7	306	CHL	C1C-C2C-CMC-OMC
24	7	306	CHL	CHA-CBD-CGD-O1D
24	7	306	CHL	CHA-CBD-CGD-O2D
24	7	310	CHL	C1C-C2C-CMC-OMC
24	7	310	CHL	C3C-C2C-CMC-OMC
24	7	312	CHL	C1C-C2C-CMC-OMC
24	7	312	CHL	C3C-C2C-CMC-OMC
24	7	312	CHL	CBD-CGD-O2D-CED
25	R	611	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	C3A-C2A-CAA-CBA
25	1	306	CLA	CHA-CBD-CGD-O1D
25	1	306	CLA	CHA-CBD-CGD-O2D
25	1	306	CLA	CAD-CBD-CGD-O1D
25	1	306	CLA	CBD-CGD-O2D-CED
25	1	313	CLA	CBD-CGD-O2D-CED
25	2	307	CLA	CBD-CGD-O2D-CED
25	2	308	CLA	CAD-CBD-CGD-O1D
25	2	308	CLA	CAD-CBD-CGD-O2D
25	2	314	CLA	CBD-CGD-O2D-CED
25	2	317	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	2	317	CLA	CHA-CBD-CGD-O2D
25	3	306	CLA	CBD-CGD-O2D-CED
25	3	307	CLA	CAD-CBD-CGD-O1D
25	3	307	CLA	CAD-CBD-CGD-O2D
25	3	307	CLA	CBD-CGD-O2D-CED
25	3	314	CLA	CHA-CBD-CGD-O1D
25	3	314	CLA	CHA-CBD-CGD-O2D
25	3	316	CLA	CHA-CBD-CGD-O1D
25	3	316	CLA	CHA-CBD-CGD-O2D
25	S	612	CLA	CBD-CGD-O2D-CED
25	S	616	CLA	C1A-C2A-CAA-CBA
25	G	308	CLA	CAD-CBD-CGD-O1D
25	G	308	CLA	CAD-CBD-CGD-O2D
25	G	314	CLA	CBD-CGD-O2D-CED
25	G	315	CLA	CBD-CGD-O2D-CED
25	9	306	CLA	CBD-CGD-O2D-CED
25	9	307	CLA	C1A-C2A-CAA-CBA
25	9	307	CLA	C3A-C2A-CAA-CBA
25	9	313	CLA	CBD-CGD-O2D-CED
25	9	314	CLA	CBD-CGD-O2D-CED
25	9	316	CLA	C4B-C3B-CAB-CBB
25	9	316	CLA	CHA-CBD-CGD-O1D
25	9	316	CLA	CHA-CBD-CGD-O2D
25	9	316	CLA	CBD-CGD-O2D-CED
25	Y	307	CLA	CHA-CBD-CGD-O1D
25	Y	307	CLA	CHA-CBD-CGD-O2D
25	Y	307	CLA	CAD-CBD-CGD-O1D
25	Y	307	CLA	CAD-CBD-CGD-O2D
25	Y	315	CLA	CHA-CBD-CGD-O1D
25	Y	315	CLA	CHA-CBD-CGD-O2D
25	8	314	CLA	CHA-CBD-CGD-O1D
25	8	314	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	601	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	601	CLA	CBD-CGD-O2D-CED
25	B	603	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C4-C3-C5-C6
25	B	604	CLA	C6-C7-C8-C9
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	B	608	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	CHA-CBD-CGD-O1D
25	B	611	CLA	CHA-CBD-CGD-O2D
25	B	613	CLA	C4-C3-C5-C6
25	B	614	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	C2-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	B	616	CLA	CHA-CBD-CGD-O2D
25	B	616	CLA	CBD-CGD-O2D-CED
25	A	604	CLA	C1A-C2A-CAA-CBA
25	A	604	CLA	CHA-CBD-CGD-O1D
25	A	604	CLA	CHA-CBD-CGD-O2D
25	A	605	CLA	CHA-CBD-CGD-O1D
25	A	605	CLA	CHA-CBD-CGD-O2D
25	C	601	CLA	CAD-CBD-CGD-O1D
25	C	601	CLA	C14-C13-C15-C16
25	C	602	CLA	CHA-CBD-CGD-O1D
25	C	602	CLA	CHA-CBD-CGD-O2D
25	C	605	CLA	CHA-CBD-CGD-O1D
25	C	605	CLA	CHA-CBD-CGD-O2D
25	C	606	CLA	CHA-CBD-CGD-O1D
25	C	606	CLA	CHA-CBD-CGD-O2D
25	C	606	CLA	CAD-CBD-CGD-O1D
25	C	606	CLA	CBD-CGD-O2D-CED
25	C	611	CLA	CHA-CBD-CGD-O1D
25	C	611	CLA	CHA-CBD-CGD-O2D
25	C	612	CLA	C1A-C2A-CAA-CBA
25	C	612	CLA	C3A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA
25	D	405	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	405	CLA	C3A-C2A-CAA-CBA
25	4	306	CLA	CHA-CBD-CGD-O1D
25	4	306	CLA	CHA-CBD-CGD-O2D
25	4	306	CLA	CAD-CBD-CGD-O1D
25	4	306	CLA	CBD-CGD-O2D-CED
25	4	313	CLA	CBD-CGD-O2D-CED
25	5	307	CLA	CBD-CGD-O2D-CED
25	5	308	CLA	CAD-CBD-CGD-O1D
25	5	308	CLA	CAD-CBD-CGD-O2D
25	5	314	CLA	CBD-CGD-O2D-CED
25	5	317	CLA	CHA-CBD-CGD-O1D
25	5	317	CLA	CHA-CBD-CGD-O2D
25	6	306	CLA	CBD-CGD-O2D-CED
25	6	307	CLA	CAD-CBD-CGD-O1D
25	6	307	CLA	CAD-CBD-CGD-O2D
25	6	314	CLA	CHA-CBD-CGD-O1D
25	6	314	CLA	CHA-CBD-CGD-O2D
25	6	316	CLA	CHA-CBD-CGD-O1D
25	6	316	CLA	CHA-CBD-CGD-O2D
25	g	308	CLA	CAD-CBD-CGD-O1D
25	g	308	CLA	CAD-CBD-CGD-O2D
25	g	315	CLA	CBD-CGD-O2D-CED
25	g	317	CLA	CBD-CGD-O2D-CED
25	u	308	CLA	C1A-C2A-CAA-CBA
25	u	308	CLA	C3A-C2A-CAA-CBA
25	u	314	CLA	CBD-CGD-O2D-CED
25	u	315	CLA	CBD-CGD-O2D-CED
25	u	315	CLA	C2-C3-C5-C6
25	u	315	CLA	C4-C3-C5-C6
25	y	308	CLA	CAD-CBD-CGD-O1D
25	y	308	CLA	CAD-CBD-CGD-O2D
25	y	316	CLA	CHA-CBD-CGD-O1D
25	y	316	CLA	CHA-CBD-CGD-O2D
25	p	308	CLA	C1A-C2A-CAA-CBA
25	p	308	CLA	C3A-C2A-CAA-CBA
25	p	314	CLA	CBD-CGD-O2D-CED
25	q	315	CLA	CHA-CBD-CGD-O1D
25	q	315	CLA	CHA-CBD-CGD-O2D
25	q	315	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	601	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C6-C7-C8-C9
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CHA-CBD-CGD-O2D
25	b	608	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	C11-C10-C8-C9
25	b	611	CLA	CHA-CBD-CGD-O1D
25	b	611	CLA	CHA-CBD-CGD-O2D
25	b	613	CLA	C4-C3-C5-C6
25	b	614	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	C4-C3-C5-C6
25	b	616	CLA	CHA-CBD-CGD-O2D
25	b	616	CLA	CBD-CGD-O2D-CED
25	a	604	CLA	C1A-C2A-CAA-CBA
25	a	604	CLA	CHA-CBD-CGD-O1D
25	a	604	CLA	CHA-CBD-CGD-O2D
25	a	605	CLA	CHA-CBD-CGD-O1D
25	a	605	CLA	CHA-CBD-CGD-O2D
25	c	601	CLA	CAD-CBD-CGD-O1D
25	c	601	CLA	C14-C13-C15-C16
25	c	602	CLA	CHA-CBD-CGD-O1D
25	c	602	CLA	CHA-CBD-CGD-O2D
25	c	605	CLA	CHA-CBD-CGD-O1D
25	c	605	CLA	CHA-CBD-CGD-O2D
25	c	606	CLA	CHA-CBD-CGD-O1D
25	c	606	CLA	CHA-CBD-CGD-O2D
25	c	606	CLA	CAD-CBD-CGD-O1D
25	c	606	CLA	CBD-CGD-O2D-CED
25	c	611	CLA	CHA-CBD-CGD-O1D
25	c	611	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	612	CLA	C1A-C2A-CAA-CBA
25	c	612	CLA	C3A-C2A-CAA-CBA
25	d	405	CLA	C1A-C2A-CAA-CBA
25	d	405	CLA	C3A-C2A-CAA-CBA
25	s	404	CLA	CBD-CGD-O2D-CED
25	s	413	CLA	CBD-CGD-O2D-CED
25	s	417	CLA	C1A-C2A-CAA-CBA
25	r	310	CLA	CBD-CGD-O2D-CED
25	r	314	CLA	C3A-C2A-CAA-CBA
25	7	308	CLA	C1A-C2A-CAA-CBA
25	7	308	CLA	C3A-C2A-CAA-CBA
25	7	314	CLA	CBD-CGD-O2D-CED
26	R	614	0IE	O1-C2-C3-C20
26	3	303	0IE	O1-C2-C30-C31
26	9	303	0IE	C14-C15-C16-C23
26	r	315	0IE	O1-C2-C3-C20
28	R	616	NEX	O24-C26-C27-C28
28	1	303	NEX	O24-C26-C27-C28
28	2	304	NEX	O24-C26-C27-C28
28	3	318	NEX	O24-C26-C27-C28
28	S	617	NEX	O24-C26-C27-C28
28	G	304	NEX	O24-C26-C27-C28
28	9	319	NEX	O24-C26-C27-C28
28	N	303	NEX	O24-C26-C27-C28
28	4	303	NEX	O24-C26-C27-C28
28	5	304	NEX	O24-C26-C27-C28
28	6	303	NEX	O24-C26-C27-C28
28	g	304	NEX	O24-C26-C27-C28
28	u	304	NEX	O24-C26-C27-C28
28	n	303	NEX	O24-C26-C27-C28
28	y	304	NEX	O24-C26-C27-C28
28	p	304	NEX	O24-C26-C27-C28
28	s	401	NEX	O24-C26-C27-C28
28	r	301	NEX	O24-C26-C27-C28
28	r	317	NEX	O24-C26-C27-C28
28	7	304	NEX	O24-C26-C27-C28
29	1	301	0UR	C5-C6-C7-C20
29	1	301	0UR	C17-C18-C19-C28
29	1	301	0UR	C17-C18-C19-C32
29	2	301	0UR	O42-C2-C3-C43
29	2	301	0UR	C5-C6-C7-C20
29	2	301	0UR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	2	301	0UR	C17-C18-C19-C28
29	2	301	0UR	C17-C18-C19-C32
29	3	301	0UR	O42-C2-C3-C43
29	G	301	0UR	O42-C2-C3-C43
29	G	301	0UR	C5-C6-C7-C20
29	G	301	0UR	C5-C6-C7-C8
29	9	301	0UR	O42-C2-C3-C43
29	9	301	0UR	C5-C6-C7-C20
29	9	301	0UR	C5-C6-C7-C8
29	N	301	0UR	O42-C2-C3-C43
29	Y	301	0UR	O42-C2-C3-C43
29	8	301	0UR	C5-C6-C7-C20
29	4	301	0UR	C5-C6-C7-C20
29	4	301	0UR	C17-C18-C19-C28
29	4	301	0UR	C17-C18-C19-C32
29	5	301	0UR	O42-C2-C3-C43
29	5	301	0UR	C5-C6-C7-C20
29	5	301	0UR	C5-C6-C7-C8
29	5	301	0UR	C17-C18-C19-C28
29	5	301	0UR	C17-C18-C19-C32
29	6	301	0UR	O42-C2-C3-C43
29	6	301	0UR	C5-C6-C7-C20
29	g	301	0UR	O42-C2-C3-C43
29	g	301	0UR	C5-C6-C7-C20
29	g	301	0UR	C5-C6-C7-C8
29	u	301	0UR	O42-C2-C3-C43
29	n	301	0UR	O42-C2-C3-C43
29	n	301	0UR	C5-C6-C7-C20
29	y	301	0UR	O42-C2-C3-C43
29	p	301	0UR	O42-C2-C3-C43
29	q	301	0UR	C5-C6-C7-C20
29	7	301	0UR	O42-C2-C3-C43
30	1	318	LHG	O1-C1-C2-C3
30	1	318	LHG	C4-O6-P-O4
30	1	318	LHG	C4-O6-P-O5
30	1	318	LHG	O7-C5-C6-O8
30	2	319	LHG	C1-C2-C3-O3
30	2	319	LHG	C3-O3-P-O4
30	2	319	LHG	C3-O3-P-O5
30	G	319	LHG	O1-C1-C2-C3
30	G	319	LHG	C4-O6-P-O4
30	G	319	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	9	318	LHG	C1-C2-C3-O3
30	9	318	LHG	O2-C2-C3-O3
30	9	318	LHG	C3-O3-P-O6
30	N	318	LHG	O1-C1-C2-O2
30	N	318	LHG	O2-C2-C3-O3
30	Y	318	LHG	C1-C2-C3-O3
30	Y	318	LHG	O10-C23-O8-C6
30	Y	318	LHG	C24-C23-O8-C6
30	A	601	LHG	C4-O6-P-O3
30	A	601	LHG	C4-O6-P-O4
30	A	601	LHG	C4-O6-P-O5
30	A	612	LHG	C3-O3-P-O5
30	C	617	LHG	C3-O3-P-O5
30	C	617	LHG	C4-O6-P-O5
30	C	617	LHG	C8-C7-O7-C5
30	D	407	LHG	O1-C1-C2-C3
30	D	407	LHG	C1-C2-C3-O3
30	D	407	LHG	O2-C2-C3-O3
30	D	407	LHG	C3-O3-P-O4
30	D	407	LHG	C3-O3-P-O5
30	D	407	LHG	C3-O3-P-O6
30	D	407	LHG	C4-O6-P-O5
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C4-O6-P-O5
30	4	318	LHG	O1-C1-C2-C3
30	4	318	LHG	C3-O3-P-O6
30	4	318	LHG	C4-O6-P-O4
30	4	318	LHG	O7-C5-C6-O8
30	5	319	LHG	C1-C2-C3-O3
30	5	319	LHG	C3-O3-P-O4
30	5	319	LHG	C3-O3-P-O5
30	g	319	LHG	O1-C1-C2-C3
30	g	319	LHG	C4-O6-P-O5
30	n	318	LHG	O2-C2-C3-O3
30	y	319	LHG	C1-C2-C3-O3
30	y	319	LHG	O10-C23-O8-C6
30	y	319	LHG	C24-C23-O8-C6
30	p	319	LHG	O1-C1-C2-C3
30	p	319	LHG	C1-C2-C3-O3
30	p	319	LHG	C4-O6-P-O3
30	p	319	LHG	C4-O6-P-O4
30	p	319	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	601	LHG	C1-C2-C3-O3
30	a	601	LHG	C4-O6-P-O3
30	a	601	LHG	C4-O6-P-O4
30	a	601	LHG	C4-O6-P-O5
30	a	612	LHG	C3-O3-P-O5
30	c	617	LHG	C3-O3-P-O5
30	c	617	LHG	C4-O6-P-O5
30	c	617	LHG	C8-C7-O7-C5
30	d	407	LHG	O1-C1-C2-C3
30	d	407	LHG	C1-C2-C3-O3
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C3-O3-P-O5
30	d	407	LHG	C3-O3-P-O6
30	d	407	LHG	C4-O6-P-O5
30	d	408	LHG	C3-O3-P-O5
30	d	408	LHG	C4-O6-P-O5
30	7	319	LHG	O1-C1-C2-C3
30	7	319	LHG	C1-C2-C3-O3
30	7	319	LHG	C4-O6-P-O3
30	7	319	LHG	C4-O6-P-O4
30	7	319	LHG	C4-O6-P-O5
31	S	615	8CT	C28-C29-C30-C31
31	S	615	8CT	C28-C29-C30-C35
31	X	601	8CT	C10-C11-C12-C13
31	X	601	8CT	C10-C11-C12-C40
31	X	601	8CT	C14-C15-C16-C17
31	X	601	8CT	C14-C15-C16-C39
31	X	601	8CT	C18-C19-C20-C21
31	V	401	8CT	C02-C03-C10-C11
31	V	401	8CT	C10-C11-C12-C13
31	V	401	8CT	C10-C11-C12-C40
31	V	401	8CT	C20-C21-C23-C24
31	V	401	8CT	C22-C21-C23-C24
31	V	401	8CT	C25-C26-C28-C29
31	V	401	8CT	C27-C26-C28-C29
31	V	401	8CT	C28-C29-C30-C31
31	T	101	8CT	C16-C17-C18-C19
31	T	101	8CT	C25-C26-C28-C29
31	T	101	8CT	C27-C26-C28-C29
31	T	101	8CT	C28-C29-C30-C35
31	B	617	8CT	C14-C15-C16-C39
31	B	617	8CT	C20-C21-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	617	8CT	C22-C21-C23-C24
31	B	617	8CT	C28-C29-C30-C35
31	A	608	8CT	C16-C17-C18-C19
31	A	608	8CT	C18-C19-C20-C21
31	C	613	8CT	C14-C15-C16-C17
31	C	613	8CT	C14-C15-C16-C39
31	C	613	8CT	C16-C17-C18-C19
31	C	613	8CT	C28-C29-C30-C31
31	C	614	8CT	C10-C11-C12-C13
31	C	614	8CT	C10-C11-C12-C40
31	C	614	8CT	C20-C21-C23-C24
31	C	614	8CT	C22-C21-C23-C24
31	C	614	8CT	C25-C26-C28-C29
31	C	614	8CT	C27-C26-C28-C29
31	C	614	8CT	C28-C29-C30-C35
31	C	615	8CT	C20-C21-C23-C24
31	C	615	8CT	C22-C21-C23-C24
31	C	615	8CT	C25-C26-C28-C29
31	C	615	8CT	C27-C26-C28-C29
31	D	410	8CT	C02-C03-C10-C11
31	D	410	8CT	C25-C26-C28-C29
31	D	410	8CT	C27-C26-C28-C29
31	D	410	8CT	C28-C29-C30-C31
31	x	601	8CT	C10-C11-C12-C13
31	x	601	8CT	C10-C11-C12-C40
31	x	601	8CT	C14-C15-C16-C17
31	x	601	8CT	C14-C15-C16-C39
31	x	601	8CT	C18-C19-C20-C21
31	v	401	8CT	C02-C03-C10-C11
31	v	401	8CT	C10-C11-C12-C13
31	v	401	8CT	C10-C11-C12-C40
31	v	401	8CT	C20-C21-C23-C24
31	v	401	8CT	C22-C21-C23-C24
31	v	401	8CT	C25-C26-C28-C29
31	v	401	8CT	C27-C26-C28-C29
31	v	401	8CT	C28-C29-C30-C31
31	t	101	8CT	C16-C17-C18-C19
31	t	101	8CT	C25-C26-C28-C29
31	t	101	8CT	C27-C26-C28-C29
31	t	101	8CT	C28-C29-C30-C35
31	b	617	8CT	C14-C15-C16-C39
31	b	617	8CT	C20-C21-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	617	8CT	C22-C21-C23-C24
31	b	617	8CT	C28-C29-C30-C35
31	a	608	8CT	C16-C17-C18-C19
31	a	608	8CT	C18-C19-C20-C21
31	c	613	8CT	C14-C15-C16-C17
31	c	613	8CT	C14-C15-C16-C39
31	c	614	8CT	C10-C11-C12-C13
31	c	614	8CT	C10-C11-C12-C40
31	c	614	8CT	C20-C21-C23-C24
31	c	614	8CT	C22-C21-C23-C24
31	c	614	8CT	C25-C26-C28-C29
31	c	614	8CT	C27-C26-C28-C29
31	c	614	8CT	C28-C29-C30-C35
31	c	615	8CT	C10-C11-C12-C13
31	c	615	8CT	C10-C11-C12-C40
31	c	615	8CT	C20-C21-C23-C24
31	c	615	8CT	C22-C21-C23-C24
31	c	615	8CT	C25-C26-C28-C29
31	c	615	8CT	C27-C26-C28-C29
31	d	410	8CT	C02-C03-C10-C11
31	d	410	8CT	C25-C26-C28-C29
31	d	410	8CT	C27-C26-C28-C29
31	d	410	8CT	C28-C29-C30-C31
31	s	416	8CT	C28-C29-C30-C31
31	s	416	8CT	C28-C29-C30-C35
32	A	609	SQD	C5-C6-S-O7
32	A	609	SQD	C5-C6-S-O8
32	A	609	SQD	C5-C6-S-O9
33	B	619	LMG	C2-C1-O1-C7
33	B	619	LMG	O6-C1-O1-C7
33	D	411	LMG	C2-C1-O1-C7
33	W	201	LMG	O6-C1-O1-C7
33	w	201	LMG	C2-C1-O1-C7
35	D	403	PHO	C2-C3-C5-C6
35	D	403	PHO	C4-C3-C5-C6
35	d	403	PHO	C2-C3-C5-C6
35	d	403	PHO	C4-C3-C5-C6
37	C	619	DGD	C2D-C1D-O3G-C3G
37	C	619	DGD	O6D-C1D-O3G-C3G
37	C	620	DGD	C2D-C1D-O3G-C3G
37	C	620	DGD	O6D-C1D-O3G-C3G
37	c	618	DGD	C2D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	c	618	DGD	O6D-C1D-O3G-C3G
39	D	406	PL9	C7-C8-C9-C11
39	D	406	PL9	C12-C13-C14-C16
39	d	406	PL9	C7-C8-C9-C11
39	d	406	PL9	C12-C13-C14-C16
25	1	306	CLA	O1D-CGD-O2D-CED
25	2	307	CLA	O1D-CGD-O2D-CED
25	S	603	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	O1D-CGD-O2D-CED
25	9	306	CLA	O1D-CGD-O2D-CED
25	8	314	CLA	O1D-CGD-O2D-CED
25	4	306	CLA	O1D-CGD-O2D-CED
25	5	307	CLA	O1D-CGD-O2D-CED
25	6	315	CLA	O1D-CGD-O2D-CED
25	u	307	CLA	O1D-CGD-O2D-CED
25	s	404	CLA	O1D-CGD-O2D-CED
25	s	413	CLA	O1D-CGD-O2D-CED
25	3	315	CLA	O1D-CGD-O2D-CED
25	9	313	CLA	O1D-CGD-O2D-CED
25	u	314	CLA	O1D-CGD-O2D-CED
25	n	307	CLA	O1D-CGD-O2D-CED
25	p	307	CLA	O1D-CGD-O2D-CED
25	p	314	CLA	O1D-CGD-O2D-CED
25	7	314	CLA	O1D-CGD-O2D-CED
24	R	607	CHL	CBD-CGD-O2D-CED
24	1	311	CHL	CBD-CGD-O2D-CED
24	1	317	CHL	CBD-CGD-O2D-CED
24	3	311	CHL	CBD-CGD-O2D-CED
24	S	607	CHL	CBD-CGD-O2D-CED
24	9	311	CHL	CBD-CGD-O2D-CED
24	Y	311	CHL	CBD-CGD-O2D-CED
24	8	309	CHL	CBD-CGD-O2D-CED
24	8	310	CHL	CBD-CGD-O2D-CED
24	4	311	CHL	CBD-CGD-O2D-CED
24	4	317	CHL	CBD-CGD-O2D-CED
24	5	311	CHL	CBD-CGD-O2D-CED
24	6	311	CHL	CBD-CGD-O2D-CED
24	g	311	CHL	CBD-CGD-O2D-CED
24	u	312	CHL	CBD-CGD-O2D-CED
24	u	313	CHL	CBD-CGD-O2D-CED
24	y	312	CHL	CBD-CGD-O2D-CED
24	p	313	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	q	310	CHL	CBD-CGD-O2D-CED
24	q	311	CHL	CBD-CGD-O2D-CED
24	s	408	CHL	CBD-CGD-O2D-CED
24	r	308	CHL	CBD-CGD-O2D-CED
25	R	609	CLA	CBD-CGD-O2D-CED
25	R	610	CLA	CBD-CGD-O2D-CED
25	1	307	CLA	CBD-CGD-O2D-CED
25	1	314	CLA	CBD-CGD-O2D-CED
25	3	313	CLA	CBD-CGD-O2D-CED
25	3	314	CLA	CBD-CGD-O2D-CED
25	3	315	CLA	CBD-CGD-O2D-CED
25	S	603	CLA	CBD-CGD-O2D-CED
25	S	611	CLA	CBD-CGD-O2D-CED
25	G	307	CLA	CBD-CGD-O2D-CED
25	N	307	CLA	CBD-CGD-O2D-CED
25	N	313	CLA	CBD-CGD-O2D-CED
25	Y	306	CLA	CBD-CGD-O2D-CED
25	Y	307	CLA	CBD-CGD-O2D-CED
25	8	314	CLA	CBD-CGD-O2D-CED
25	C	611	CLA	CBD-CGD-O2D-CED
25	4	307	CLA	CBD-CGD-O2D-CED
25	4	314	CLA	CBD-CGD-O2D-CED
25	6	313	CLA	CBD-CGD-O2D-CED
25	6	315	CLA	CBD-CGD-O2D-CED
25	g	307	CLA	CBD-CGD-O2D-CED
25	g	314	CLA	CBD-CGD-O2D-CED
25	u	307	CLA	CBD-CGD-O2D-CED
25	u	317	CLA	CBD-CGD-O2D-CED
25	n	307	CLA	CBD-CGD-O2D-CED
25	n	313	CLA	CBD-CGD-O2D-CED
25	y	307	CLA	CBD-CGD-O2D-CED
25	p	307	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	c	611	CLA	CBD-CGD-O2D-CED
25	s	412	CLA	CBD-CGD-O2D-CED
25	r	311	CLA	CBD-CGD-O2D-CED
25	r	312	CLA	CBD-CGD-O2D-CED
25	7	307	CLA	CBD-CGD-O2D-CED
25	A	603	CLA	O1A-CGA-O2A-C1
25	a	603	CLA	O1A-CGA-O2A-C1
30	D	408	LHG	O10-C23-O8-C6
30	d	408	LHG	O10-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	C	620	DGD	C4E-C5E-C6E-O5E
24	p	312	CHL	O1D-CGD-O2D-CED
25	1	313	CLA	O1D-CGD-O2D-CED
25	3	306	CLA	O1D-CGD-O2D-CED
25	G	314	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
25	6	306	CLA	O1D-CGD-O2D-CED
25	q	315	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
24	2	312	CHL	O1D-CGD-O2D-CED
24	G	312	CHL	O1D-CGD-O2D-CED
24	Y	311	CHL	O1D-CGD-O2D-CED
24	g	312	CHL	O1D-CGD-O2D-CED
24	y	312	CHL	O1D-CGD-O2D-CED
24	7	312	CHL	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	2	314	CLA	O1D-CGD-O2D-CED
25	9	314	CLA	O1D-CGD-O2D-CED
25	9	316	CLA	O1D-CGD-O2D-CED
25	N	307	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
25	4	313	CLA	O1D-CGD-O2D-CED
25	g	315	CLA	O1D-CGD-O2D-CED
25	g	317	CLA	O1D-CGD-O2D-CED
25	u	315	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
25	c	606	CLA	O1D-CGD-O2D-CED
25	r	312	CLA	O1D-CGD-O2D-CED
25	7	307	CLA	O1D-CGD-O2D-CED
25	A	603	CLA	CBA-CGA-O2A-C1
25	a	603	CLA	CBA-CGA-O2A-C1
30	D	408	LHG	C24-C23-O8-C6
30	d	408	LHG	C24-C23-O8-C6
37	c	619	DGD	C4E-C5E-C6E-O5E
24	R	608	CHL	CBD-CGD-O2D-CED
24	2	305	CHL	CBD-CGD-O2D-CED
24	2	306	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2	311	CHL	CBD-CGD-O2D-CED
24	3	304	CHL	CBD-CGD-O2D-CED
24	S	606	CHL	CBD-CGD-O2D-CED
24	N	305	CHL	CBD-CGD-O2D-CED
24	5	305	CHL	CBD-CGD-O2D-CED
24	6	304	CHL	CBD-CGD-O2D-CED
24	n	305	CHL	CBD-CGD-O2D-CED
24	n	308	CHL	CBD-CGD-O2D-CED
24	s	403	CHL	CBD-CGD-O2D-CED
24	s	407	CHL	CBD-CGD-O2D-CED
24	r	309	CHL	CBD-CGD-O2D-CED
24	7	313	CHL	CBD-CGD-O2D-CED
25	1	315	CLA	CBD-CGD-O2D-CED
25	2	317	CLA	CBD-CGD-O2D-CED
25	S	616	CLA	CBD-CGD-O2D-CED
25	N	315	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	A	603	CLA	CBD-CGD-O2D-CED
25	A	610	CLA	CBD-CGD-O2D-CED
25	C	601	CLA	CBD-CGD-O2D-CED
25	C	603	CLA	CBD-CGD-O2D-CED
25	5	317	CLA	CBD-CGD-O2D-CED
25	6	307	CLA	CBD-CGD-O2D-CED
25	6	314	CLA	CBD-CGD-O2D-CED
25	n	315	CLA	CBD-CGD-O2D-CED
25	p	315	CLA	CBD-CGD-O2D-CED
25	q	313	CLA	CBD-CGD-O2D-CED
25	b	607	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	a	603	CLA	CBD-CGD-O2D-CED
25	a	610	CLA	CBD-CGD-O2D-CED
25	c	601	CLA	CBD-CGD-O2D-CED
25	c	603	CLA	CBD-CGD-O2D-CED
25	7	315	CLA	CBD-CGD-O2D-CED
25	c	612	CLA	O1A-CGA-O2A-C1
30	p	319	LHG	O10-C23-O8-C6
30	7	319	LHG	O10-C23-O8-C6
24	G	311	CHL	O1D-CGD-O2D-CED
24	5	312	CHL	O1D-CGD-O2D-CED
25	G	315	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	5	314	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
24	9	312	CHL	O1D-CGD-O2D-CED
24	N	311	CHL	O1D-CGD-O2D-CED
25	3	307	CLA	O1D-CGD-O2D-CED
25	C	606	CLA	O1D-CGD-O2D-CED
24	1	310	CHL	CBD-CGD-O2D-CED
24	S	602	CHL	CBD-CGD-O2D-CED
24	G	306	CHL	CBD-CGD-O2D-CED
24	9	305	CHL	CBD-CGD-O2D-CED
24	5	306	CHL	CBD-CGD-O2D-CED
24	5	309	CHL	CBD-CGD-O2D-CED
24	u	306	CHL	CBD-CGD-O2D-CED
24	y	313	CHL	CBD-CGD-O2D-CED
24	s	402	CHL	CBD-CGD-O2D-CED
25	G	317	CLA	CBD-CGD-O2D-CED
25	s	410	CLA	CBD-CGD-O2D-CED
25	s	417	CLA	CBD-CGD-O2D-CED
24	n	311	CHL	O1D-CGD-O2D-CED
25	r	310	CLA	O1D-CGD-O2D-CED
30	9	318	LHG	O9-C7-O7-C5
25	3	313	CLA	O1D-CGD-O2D-CED
29	9	301	0UR	O57-C45-O44-C43
24	Y	310	CHL	C3-C5-C6-C7
24	p	305	CHL	C3-C5-C6-C7
24	7	305	CHL	C3-C5-C6-C7
25	2	315	CLA	C3-C5-C6-C7
25	G	315	CLA	C3-C5-C6-C7
25	9	314	CLA	C3-C5-C6-C7
25	N	314	CLA	C3-C5-C6-C7
25	Y	314	CLA	C3-C5-C6-C7
25	8	312	CLA	C3-C5-C6-C7
25	B	612	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	C	611	CLA	C3-C5-C6-C7
25	C	612	CLA	C3-C5-C6-C7
25	5	315	CLA	C3-C5-C6-C7
25	g	315	CLA	C3-C5-C6-C7
25	u	315	CLA	C3-C5-C6-C7
25	y	315	CLA	C3-C5-C6-C7
25	q	313	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C3-C5-C6-C7
25	b	612	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	c	611	CLA	C3-C5-C6-C7
35	A	606	PHO	C3-C5-C6-C7
35	a	606	PHO	C3-C5-C6-C7
25	N	307	CLA	CBA-CGA-O2A-C1
25	A	604	CLA	CBA-CGA-O2A-C1
25	n	307	CLA	CBA-CGA-O2A-C1
25	a	604	CLA	CBA-CGA-O2A-C1
30	N	318	LHG	C24-C23-O8-C6
30	n	318	LHG	C24-C23-O8-C6
30	p	319	LHG	C24-C23-O8-C6
30	7	319	LHG	C24-C23-O8-C6
33	B	619	LMG	C29-C28-O8-C9
29	9	301	0UR	C46-C45-O44-C43
29	u	301	0UR	C46-C45-O44-C43
30	9	318	LHG	C8-C7-O7-C5
24	3	311	CHL	O1D-CGD-O2D-CED
24	8	309	CHL	O1D-CGD-O2D-CED
24	g	311	CHL	O1D-CGD-O2D-CED
24	u	313	CHL	O1D-CGD-O2D-CED
24	q	310	CHL	O1D-CGD-O2D-CED
25	6	313	CLA	O1D-CGD-O2D-CED
25	g	307	CLA	O1D-CGD-O2D-CED
25	u	317	CLA	O1D-CGD-O2D-CED
24	N	304	CHL	CBD-CGD-O2D-CED
24	Y	312	CHL	CBD-CGD-O2D-CED
24	4	310	CHL	CBD-CGD-O2D-CED
24	4	312	CHL	CBD-CGD-O2D-CED
24	g	306	CHL	CBD-CGD-O2D-CED
24	n	304	CHL	CBD-CGD-O2D-CED
24	y	310	CHL	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	4	315	CLA	CBD-CGD-O2D-CED
25	y	308	CLA	CBD-CGD-O2D-CED
25	C	612	CLA	O1A-CGA-O2A-C1
37	C	620	DGD	O6E-C5E-C6E-O5E
25	C	603	CLA	C4-C3-C5-C6
25	c	603	CLA	C4-C3-C5-C6
39	D	406	PL9	C20-C19-C21-C22
39	d	406	PL9	C20-C19-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C2-C3-C5-C6
25	b	613	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
24	1	309	CHL	CBD-CGD-O2D-CED
24	1	312	CHL	CBD-CGD-O2D-CED
24	3	305	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	CBD-CGD-O2D-CED
24	Y	309	CHL	CBD-CGD-O2D-CED
24	6	305	CHL	CBD-CGD-O2D-CED
24	g	313	CHL	CBD-CGD-O2D-CED
24	g	318	CHL	CBD-CGD-O2D-CED
24	p	305	CHL	CBD-CGD-O2D-CED
24	q	303	CHL	CBD-CGD-O2D-CED
25	R	613	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
25	9	307	CLA	CBD-CGD-O2D-CED
25	8	312	CLA	CBD-CGD-O2D-CED
25	D	405	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
24	R	601	CHL	C2A-CAA-CBA-CGA
24	S	605	CHL	C2A-CAA-CBA-CGA
24	S	607	CHL	C2A-CAA-CBA-CGA
24	9	309	CHL	C2A-CAA-CBA-CGA
24	N	311	CHL	C2A-CAA-CBA-CGA
24	Y	311	CHL	C2A-CAA-CBA-CGA
24	8	303	CHL	C2A-CAA-CBA-CGA
24	8	308	CHL	C2A-CAA-CBA-CGA
24	u	306	CHL	C2A-CAA-CBA-CGA
24	u	310	CHL	C2A-CAA-CBA-CGA
24	n	304	CHL	C2A-CAA-CBA-CGA
24	y	310	CHL	C2A-CAA-CBA-CGA
24	y	312	CHL	C2A-CAA-CBA-CGA
24	p	312	CHL	C2A-CAA-CBA-CGA
24	q	303	CHL	C2A-CAA-CBA-CGA
24	q	308	CHL	C2A-CAA-CBA-CGA
24	r	302	CHL	C2A-CAA-CBA-CGA
24	7	312	CHL	C2A-CAA-CBA-CGA
25	Y	307	CLA	C2A-CAA-CBA-CGA
25	8	305	CLA	C2A-CAA-CBA-CGA
25	q	305	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C2A-CAA-CBA-CGA
33	D	411	LMG	O10-C28-O8-C9
24	6	311	CHL	O1D-CGD-O2D-CED
30	1	318	LHG	C24-C25-C26-C27
30	2	319	LHG	C24-C25-C26-C27
30	G	319	LHG	C24-C25-C26-C27
30	9	318	LHG	C24-C25-C26-C27
30	N	318	LHG	C24-C25-C26-C27
30	Y	318	LHG	C24-C25-C26-C27
30	A	612	LHG	C24-C25-C26-C27
30	C	617	LHG	C24-C25-C26-C27
30	D	407	LHG	C24-C25-C26-C27
30	D	408	LHG	C24-C25-C26-C27
30	4	318	LHG	C24-C25-C26-C27
30	5	319	LHG	C24-C25-C26-C27
30	g	319	LHG	C24-C25-C26-C27
30	n	318	LHG	C24-C25-C26-C27
30	y	319	LHG	C24-C25-C26-C27
30	p	319	LHG	C24-C25-C26-C27
30	a	612	LHG	C24-C25-C26-C27
30	c	617	LHG	C24-C25-C26-C27
30	d	407	LHG	C24-C25-C26-C27
30	7	319	LHG	C24-C25-C26-C27
24	8	304	CHL	C3-C5-C6-C7
24	g	306	CHL	C3-C5-C6-C7
24	y	306	CHL	C3-C5-C6-C7
24	y	311	CHL	C3-C5-C6-C7
24	q	304	CHL	C3-C5-C6-C7
25	B	602	CLA	C3-C5-C6-C7
25	B	608	CLA	C3-C5-C6-C7
25	B	609	CLA	C3-C5-C6-C7
25	c	612	CLA	C3-C5-C6-C7
25	9	314	CLA	CBA-CGA-O2A-C1
25	B	606	CLA	CBA-CGA-O2A-C1
25	C	612	CLA	CBA-CGA-O2A-C1
25	p	315	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	CBA-CGA-O2A-C1
25	c	604	CLA	CBA-CGA-O2A-C1
25	c	612	CLA	CBA-CGA-O2A-C1
30	G	319	LHG	C24-C23-O8-C6
37	c	619	DGD	O6E-C5E-C6E-O5E
33	d	411	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	s	408	CHL	O1D-CGD-O2D-CED
25	G	307	CLA	O1D-CGD-O2D-CED
25	g	314	CLA	O1D-CGD-O2D-CED
24	2	309	CHL	CBD-CGD-O2D-CED
24	G	313	CHL	CBD-CGD-O2D-CED
24	G	318	CHL	CBD-CGD-O2D-CED
24	Y	308	CHL	CBD-CGD-O2D-CED
24	8	304	CHL	CBD-CGD-O2D-CED
24	q	304	CHL	CBD-CGD-O2D-CED
25	C	602	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	c	602	CLA	CBD-CGD-O2D-CED
33	w	201	LMG	C15-C16-C17-C18
24	R	607	CHL	O1D-CGD-O2D-CED
24	r	308	CHL	O1D-CGD-O2D-CED
25	R	609	CLA	O1D-CGD-O2D-CED
25	R	610	CLA	O1D-CGD-O2D-CED
25	Y	306	CLA	O1D-CGD-O2D-CED
25	C	611	CLA	O1D-CGD-O2D-CED
25	y	307	CLA	O1D-CGD-O2D-CED
25	c	611	CLA	O1D-CGD-O2D-CED
30	C	617	LHG	O9-C7-O7-C5
30	c	617	LHG	O9-C7-O7-C5
32	D	409	SQD	O49-C7-O47-C45
32	d	409	SQD	O49-C7-O47-C45
25	B	606	CLA	O1A-CGA-O2A-C1
25	A	604	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	O1A-CGA-O2A-C1
30	G	319	LHG	O10-C23-O8-C6
30	N	318	LHG	O10-C23-O8-C6
30	g	319	LHG	O10-C23-O8-C6
30	n	318	LHG	O10-C23-O8-C6
32	a	609	SQD	O10-C23-O48-C46
24	1	317	CHL	O1D-CGD-O2D-CED
24	4	317	CHL	O1D-CGD-O2D-CED
31	C	614	8CT	C12-C13-C14-C15
31	C	615	8CT	C16-C17-C18-C19
31	C	615	8CT	C23-C24-C25-C26
31	c	613	8CT	C16-C17-C18-C19
31	c	614	8CT	C12-C13-C14-C15
31	c	615	8CT	C16-C17-C18-C19
24	R	605	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2	310	CHL	CBD-CGD-O2D-CED
24	3	309	CHL	CBD-CGD-O2D-CED
24	S	605	CHL	CBD-CGD-O2D-CED
24	G	305	CHL	CBD-CGD-O2D-CED
24	N	310	CHL	CBD-CGD-O2D-CED
24	Y	304	CHL	CBD-CGD-O2D-CED
24	8	303	CHL	CBD-CGD-O2D-CED
24	4	309	CHL	CBD-CGD-O2D-CED
24	5	310	CHL	CBD-CGD-O2D-CED
24	6	308	CHL	CBD-CGD-O2D-CED
24	6	312	CHL	CBD-CGD-O2D-CED
24	g	305	CHL	CBD-CGD-O2D-CED
24	u	305	CHL	CBD-CGD-O2D-CED
24	y	309	CHL	CBD-CGD-O2D-CED
24	s	406	CHL	CBD-CGD-O2D-CED
24	r	307	CHL	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	2	308	CLA	CBD-CGD-O2D-CED
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	5	308	CLA	CBD-CGD-O2D-CED
25	6	316	CLA	CBD-CGD-O2D-CED
25	u	308	CLA	CBD-CGD-O2D-CED
25	n	306	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	CBD-CGD-O2D-CED
25	c	604	CLA	CBD-CGD-O2D-CED
25	d	405	CLA	CBD-CGD-O2D-CED
25	s	411	CLA	CBD-CGD-O2D-CED
25	r	304	CLA	CBD-CGD-O2D-CED
25	r	314	CLA	CBD-CGD-O2D-CED
24	S	607	CHL	O1D-CGD-O2D-CED
25	1	314	CLA	O1D-CGD-O2D-CED
25	r	311	CLA	O1D-CGD-O2D-CED
29	1	301	0UR	O57-C45-O44-C43
29	2	301	0UR	O57-C45-O44-C43
29	3	301	0UR	O57-C45-O44-C43
29	G	301	0UR	O57-C45-O44-C43
29	N	301	0UR	O57-C45-O44-C43
29	Y	301	0UR	O57-C45-O44-C43
29	8	301	0UR	O57-C45-O44-C43
29	4	301	0UR	O57-C45-O44-C43
29	5	301	0UR	O57-C45-O44-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	6	301	0UR	O57-C45-O44-C43
29	g	301	0UR	O57-C45-O44-C43
29	u	301	0UR	O57-C45-O44-C43
29	n	301	0UR	O57-C45-O44-C43
29	y	301	0UR	O57-C45-O44-C43
29	p	301	0UR	O57-C45-O44-C43
29	q	301	0UR	O57-C45-O44-C43
29	7	301	0UR	O57-C45-O44-C43
30	2	319	LHG	O2-C2-C3-O3
30	Y	318	LHG	O2-C2-C3-O3
30	5	319	LHG	O2-C2-C3-O3
30	y	319	LHG	O2-C2-C3-O3
30	p	319	LHG	O2-C2-C3-O3
30	d	407	LHG	O2-C2-C3-O3
30	d	408	LHG	O2-C2-C3-O3
30	7	319	LHG	O2-C2-C3-O3
24	G	306	CHL	C3-C5-C6-C7
24	Y	305	CHL	C3-C5-C6-C7
24	n	305	CHL	C3-C5-C6-C7
25	n	314	CLA	C3-C5-C6-C7
25	b	609	CLA	C3-C5-C6-C7
25	C	604	CLA	CBA-CGA-O2A-C1
25	7	315	CLA	CBA-CGA-O2A-C1
30	9	318	LHG	C24-C23-O8-C6
33	D	411	LMG	C29-C28-O8-C9
33	m	101	LMG	C29-C28-O8-C9
25	N	307	CLA	O1A-CGA-O2A-C1
25	n	307	CLA	O1A-CGA-O2A-C1
25	a	604	CLA	O1A-CGA-O2A-C1
33	B	619	LMG	O10-C28-O8-C9
29	1	301	0UR	C46-C45-O44-C43
29	2	301	0UR	C46-C45-O44-C43
29	3	301	0UR	C46-C45-O44-C43
29	G	301	0UR	C46-C45-O44-C43
29	N	301	0UR	C46-C45-O44-C43
29	Y	301	0UR	C46-C45-O44-C43
29	8	301	0UR	C46-C45-O44-C43
29	4	301	0UR	C46-C45-O44-C43
29	5	301	0UR	C46-C45-O44-C43
29	6	301	0UR	C46-C45-O44-C43
29	g	301	0UR	C46-C45-O44-C43
29	n	301	0UR	C46-C45-O44-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	y	301	0UR	C46-C45-O44-C43
29	p	301	0UR	C46-C45-O44-C43
29	q	301	0UR	C46-C45-O44-C43
29	7	301	0UR	C46-C45-O44-C43
24	9	311	CHL	O1D-CGD-O2D-CED
25	S	611	CLA	O1D-CGD-O2D-CED
25	n	313	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	s	412	CLA	O1D-CGD-O2D-CED
32	D	409	SQD	C8-C7-O47-C45
32	d	409	SQD	C8-C7-O47-C45
24	R	606	CHL	CBD-CGD-O2D-CED
24	u	311	CHL	CBD-CGD-O2D-CED
24	n	312	CHL	CBD-CGD-O2D-CED
24	7	305	CHL	CBD-CGD-O2D-CED
25	S	610	CLA	CBD-CGD-O2D-CED
25	Y	313	CLA	CBD-CGD-O2D-CED
25	C	604	CLA	CBD-CGD-O2D-CED
33	D	411	LMG	C16-C17-C18-C19
37	C	619	DGD	C5B-C6B-C7B-C8B
37	C	620	DGD	C6B-C7B-C8B-C9B
25	3	314	CLA	O1D-CGD-O2D-CED
29	2	301	0UR	O44-C45-C46-C47
29	9	301	0UR	O44-C45-C46-C47
29	5	301	0UR	O44-C45-C46-C47
29	u	301	0UR	O44-C45-C46-C47
29	p	301	0UR	O44-C45-C46-C47
29	7	301	0UR	O44-C45-C46-C47
30	5	319	LHG	C14-C15-C16-C17
33	C	618	LMG	C12-C13-C14-C15
33	C	618	LMG	C29-C30-C31-C32
33	m	101	LMG	C13-C14-C15-C16
33	d	401	LMG	C11-C12-C13-C14
37	c	618	DGD	C5B-C6B-C7B-C8B
24	8	310	CHL	O1D-CGD-O2D-CED
25	Y	307	CLA	O1D-CGD-O2D-CED
25	4	307	CLA	O1D-CGD-O2D-CED
30	5	319	LHG	C12-C13-C14-C15
30	d	408	LHG	C24-C25-C26-C27
37	c	619	DGD	C6B-C7B-C8B-C9B
24	9	310	CHL	CBD-CGD-O2D-CED
25	u	315	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	g	319	LHG	C24-C23-O8-C6
24	1	311	CHL	O1D-CGD-O2D-CED
24	4	311	CHL	O1D-CGD-O2D-CED
24	u	312	CHL	O1D-CGD-O2D-CED
24	q	311	CHL	O1D-CGD-O2D-CED
25	N	313	CLA	O1D-CGD-O2D-CED
37	C	619	DGD	C4E-C5E-C6E-O5E
33	B	619	LMG	C13-C14-C15-C16
25	9	314	CLA	O1A-CGA-O2A-C1
25	C	604	CLA	O1A-CGA-O2A-C1
25	p	315	CLA	O1A-CGA-O2A-C1
25	7	315	CLA	O1A-CGA-O2A-C1
33	m	101	LMG	O10-C28-O8-C9
30	d	408	LHG	C11-C10-C9-C8
33	C	618	LMG	C14-C15-C16-C17
39	D	406	PL9	C47-C48-C49-C51
39	d	406	PL9	C47-C48-C49-C51
25	9	314	CLA	C4-C3-C5-C6
25	B	612	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	9	314	CLA	C2-C3-C5-C6
25	B	612	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
24	2	318	CHL	CBD-CGD-O2D-CED
24	n	317	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	C2A-CAA-CBA-CGA
24	2	312	CHL	C2A-CAA-CBA-CGA
24	9	305	CHL	C2A-CAA-CBA-CGA
24	N	304	CHL	C2A-CAA-CBA-CGA
24	Y	309	CHL	C2A-CAA-CBA-CGA
24	5	312	CHL	C2A-CAA-CBA-CGA
24	6	309	CHL	C2A-CAA-CBA-CGA
24	n	309	CHL	C2A-CAA-CBA-CGA
24	s	402	CHL	C2A-CAA-CBA-CGA
24	s	406	CHL	C2A-CAA-CBA-CGA
24	s	408	CHL	C2A-CAA-CBA-CGA
25	B	614	CLA	C2A-CAA-CBA-CGA
25	y	308	CLA	C2A-CAA-CBA-CGA
24	p	313	CHL	O1D-CGD-O2D-CED
30	2	319	LHG	C12-C13-C14-C15
33	D	401	LMG	C14-C15-C16-C17
33	m	101	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	w	201	LMG	O6-C5-C6-O5
33	d	411	LMG	O6-C5-C6-O5
37	C	619	DGD	O6E-C5E-C6E-O5E
25	c	604	CLA	O1A-CGA-O2A-C1
30	9	318	LHG	O10-C23-O8-C6
33	C	618	LMG	O6-C1-O1-C7
33	w	201	LMG	O6-C1-O1-C7
25	Y	307	CLA	CBA-CGA-O2A-C1
33	B	619	LMG	C29-C30-C31-C32
37	C	620	DGD	C2B-C3B-C4B-C5B
24	u	309	CHL	CBD-CGD-O2D-CED
24	y	305	CHL	CBD-CGD-O2D-CED
25	B	602	CLA	CBD-CGD-O2D-CED
25	1	307	CLA	O1D-CGD-O2D-CED
37	c	618	DGD	C4E-C5E-C6E-O5E
29	1	301	0UR	O44-C45-C46-C47
29	3	301	0UR	O44-C45-C46-C47
29	G	301	0UR	O44-C45-C46-C47
29	8	301	0UR	O44-C45-C46-C47
29	4	301	0UR	O44-C45-C46-C47
29	6	301	0UR	O44-C45-C46-C47
29	g	301	0UR	O44-C45-C46-C47
29	n	301	0UR	O44-C45-C46-C47
29	q	301	0UR	O44-C45-C46-C47
24	5	311	CHL	O1D-CGD-O2D-CED
25	C	603	CLA	O1D-CGD-O2D-CED
25	4	314	CLA	O1D-CGD-O2D-CED
25	c	603	CLA	O1D-CGD-O2D-CED
25	u	315	CLA	O1A-CGA-O2A-C1
24	n	308	CHL	O1D-CGD-O2D-CED
24	7	313	CHL	O1D-CGD-O2D-CED
25	5	317	CLA	O1D-CGD-O2D-CED
25	6	307	CLA	O1D-CGD-O2D-CED
24	3	312	CHL	CBD-CGD-O2D-CED
24	N	312	CHL	CBD-CGD-O2D-CED
24	6	309	CHL	CBD-CGD-O2D-CED
24	n	310	CHL	CBD-CGD-O2D-CED
25	q	313	CLA	O1D-CGD-O2D-CED
30	N	318	LHG	C1-C2-C3-O3
30	A	601	LHG	C1-C2-C3-O3
30	D	408	LHG	C1-C2-C3-O3
30	n	318	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C1-C2-C3-O3
25	c	610	CLA	C3-C5-C6-C7
24	2	311	CHL	O1D-CGD-O2D-CED
25	2	317	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	O1D-CGD-O2D-CED
25	p	315	CLA	O1D-CGD-O2D-CED
24	G	311	CHL	CBA-CGA-O2A-C1
24	9	305	CHL	CBA-CGA-O2A-C1
24	N	305	CHL	CBA-CGA-O2A-C1
24	Y	310	CHL	CBA-CGA-O2A-C1
24	g	311	CHL	CBA-CGA-O2A-C1
24	u	306	CHL	CBA-CGA-O2A-C1
25	Y	314	CLA	CBA-CGA-O2A-C1
25	C	605	CLA	CBA-CGA-O2A-C1
25	C	610	CLA	CBA-CGA-O2A-C1
25	D	405	CLA	CBA-CGA-O2A-C1
25	y	308	CLA	CBA-CGA-O2A-C1
25	y	315	CLA	CBA-CGA-O2A-C1
25	c	610	CLA	CBA-CGA-O2A-C1
25	d	405	CLA	CBA-CGA-O2A-C1
30	D	407	LHG	C24-C23-O8-C6
30	d	407	LHG	C24-C23-O8-C6
32	a	609	SQD	C24-C23-O48-C46
33	W	201	LMG	C29-C28-O8-C9
33	w	201	LMG	C29-C28-O8-C9
24	3	308	CHL	CBD-CGD-O2D-CED
24	9	304	CHL	CBD-CGD-O2D-CED
24	9	308	CHL	CBD-CGD-O2D-CED
25	N	306	CLA	CBD-CGD-O2D-CED
25	q	312	CLA	CBD-CGD-O2D-CED
33	d	411	LMG	C4-C5-C6-O5
33	B	619	LMG	C15-C16-C17-C18
33	m	101	LMG	C15-C16-C17-C18
31	X	601	8CT	C16-C17-C18-C19
31	T	101	8CT	C18-C19-C20-C21
31	B	617	8CT	C16-C17-C18-C19
31	x	601	8CT	C16-C17-C18-C19
31	t	101	8CT	C18-C19-C20-C21
31	b	617	8CT	C16-C17-C18-C19
31	c	615	8CT	C23-C24-C25-C26
33	D	411	LMG	C28-C29-C30-C31
30	1	318	LHG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	4	318	LHG	C14-C15-C16-C17
25	u	307	CLA	C5-C6-C7-C8
25	c	603	CLA	C15-C16-C17-C18
24	g	311	CHL	O1A-CGA-O2A-C1
33	D	411	LMG	C12-C13-C14-C15
24	u	318	CHL	CBD-CGD-O2D-CED
29	N	301	0UR	O44-C45-C46-C47
33	D	411	LMG	C14-C15-C16-C17
24	G	305	CHL	C15-C16-C17-C18
24	G	313	CHL	C5-C6-C7-C8
24	9	304	CHL	C13-C15-C16-C17
24	g	306	CHL	C8-C10-C11-C12
24	g	313	CHL	C5-C6-C7-C8
24	y	305	CHL	C8-C10-C11-C12
24	7	306	CHL	C10-C11-C12-C13
25	B	609	CLA	C8-C10-C11-C12
25	b	603	CLA	C13-C15-C16-C17
32	a	609	SQD	C2-C1-O6-C44
33	m	101	LMG	C2-C1-O1-C7
37	c	618	DGD	O6E-C5E-C6E-O5E
25	C	603	CLA	C2-C3-C5-C6
25	c	603	CLA	C2-C3-C5-C6
39	d	406	PL9	C12-C11-C9-C8
24	G	306	CHL	C11-C12-C13-C14
24	9	305	CHL	C14-C13-C15-C16
24	Y	305	CHL	C6-C7-C8-C9
24	Y	305	CHL	C11-C12-C13-C14
24	Y	312	CHL	C11-C12-C13-C14
24	8	304	CHL	C6-C7-C8-C9
24	g	306	CHL	C11-C12-C13-C14
24	u	306	CHL	C14-C13-C15-C16
24	n	305	CHL	C6-C7-C8-C9
24	y	306	CHL	C6-C7-C8-C9
24	y	306	CHL	C11-C12-C13-C14
24	y	313	CHL	C11-C12-C13-C14
24	p	305	CHL	C11-C12-C13-C14
24	p	306	CHL	C6-C7-C8-C9
24	p	306	CHL	C11-C12-C13-C14
24	q	304	CHL	C6-C7-C8-C9
24	7	305	CHL	C11-C12-C13-C14
24	7	306	CHL	C6-C7-C8-C9
24	7	306	CHL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C12-C13-C14
25	B	605	CLA	C14-C13-C15-C16
25	B	609	CLA	C11-C10-C8-C9
25	A	604	CLA	C14-C13-C15-C16
25	C	608	CLA	C11-C12-C13-C14
25	p	315	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C12-C13-C14
25	b	605	CLA	C14-C13-C15-C16
25	a	604	CLA	C14-C13-C15-C16
25	c	608	CLA	C11-C12-C13-C14
35	A	606	PHO	C14-C13-C15-C16
35	a	606	PHO	C14-C13-C15-C16
24	S	606	CHL	O1D-CGD-O2D-CED
24	N	305	CHL	O1D-CGD-O2D-CED
24	6	304	CHL	O1D-CGD-O2D-CED
25	S	616	CLA	O1D-CGD-O2D-CED
25	N	315	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	O1D-CGD-O2D-CED
25	6	314	CLA	O1D-CGD-O2D-CED
25	b	607	CLA	O1D-CGD-O2D-CED
25	a	610	CLA	O1D-CGD-O2D-CED
24	N	317	CHL	CBD-CGD-O2D-CED
24	5	318	CHL	CBD-CGD-O2D-CED
24	N	312	CHL	C5-C6-C7-C8
24	Y	305	CHL	C10-C11-C12-C13
24	g	305	CHL	C15-C16-C17-C18
24	n	312	CHL	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	C	603	CLA	C15-C16-C17-C18
24	S	601	CHL	C2A-CAA-CBA-CGA
24	N	305	CHL	C2A-CAA-CBA-CGA
24	u	312	CHL	C2A-CAA-CBA-CGA
24	r	308	CHL	C2A-CAA-CBA-CGA
25	B	601	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C2A-CAA-CBA-CGA
26	9	303	0IE	C22-C12-C13-C14
29	2	301	0UR	C22-C16-C17-C18
29	N	301	0UR	C5-C6-C7-C20
29	Y	301	0UR	C5-C6-C7-C20
29	5	301	0UR	C22-C16-C17-C18
29	u	301	0UR	C5-C6-C7-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	y	301	0UR	C5-C6-C7-C20
31	S	615	8CT	C22-C21-C23-C24
31	X	601	8CT	C27-C26-C28-C29
31	T	101	8CT	C10-C11-C12-C40
31	T	101	8CT	C14-C15-C16-C39
31	B	617	8CT	C27-C26-C28-C29
31	A	608	8CT	C10-C11-C12-C40
31	A	608	8CT	C14-C15-C16-C39
31	C	613	8CT	C10-C11-C12-C40
31	C	615	8CT	C14-C15-C16-C39
31	x	601	8CT	C27-C26-C28-C29
31	t	101	8CT	C10-C11-C12-C40
31	b	617	8CT	C27-C26-C28-C29
31	a	608	8CT	C10-C11-C12-C40
31	a	608	8CT	C14-C15-C16-C39
31	c	613	8CT	C10-C11-C12-C40
31	c	615	8CT	C14-C15-C16-C39
31	s	416	8CT	C22-C21-C23-C24
29	1	301	0UR	O57-C45-C46-C47
29	2	301	0UR	O57-C45-C46-C47
29	9	301	0UR	O57-C45-C46-C47
29	4	301	0UR	O57-C45-C46-C47
29	5	301	0UR	O57-C45-C46-C47
29	6	301	0UR	O57-C45-C46-C47
29	u	301	0UR	O57-C45-C46-C47
29	p	301	0UR	O57-C45-C46-C47
29	7	301	0UR	O57-C45-C46-C47
29	2	301	0UR	C15-C16-C17-C18
29	5	301	0UR	C15-C16-C17-C18
31	T	101	8CT	C10-C11-C12-C13
31	T	101	8CT	C14-C15-C16-C17
31	B	617	8CT	C14-C15-C16-C17
31	A	608	8CT	C10-C11-C12-C13
31	A	608	8CT	C14-C15-C16-C17
31	C	613	8CT	C10-C11-C12-C13
31	C	615	8CT	C14-C15-C16-C17
31	t	101	8CT	C10-C11-C12-C13
31	t	101	8CT	C14-C15-C16-C17
31	b	617	8CT	C10-C11-C12-C13
31	b	617	8CT	C14-C15-C16-C17
31	a	608	8CT	C10-C11-C12-C13
31	a	608	8CT	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	613	8CT	C10-C11-C12-C13
31	c	615	8CT	C14-C15-C16-C17
25	7	315	CLA	O1D-CGD-O2D-CED
33	C	618	LMG	C33-C34-C35-C36
33	w	201	LMG	C4-C5-C6-O5
25	C	610	CLA	O1A-CGA-O2A-C1
25	c	610	CLA	O1A-CGA-O2A-C1
24	g	305	CHL	C13-C15-C16-C17
24	s	407	CHL	O1D-CGD-O2D-CED
30	A	612	LHG	C31-C32-C33-C34
37	C	619	DGD	C4D-C5D-C6D-O5D
24	4	304	CHL	CBD-CGD-O2D-CED
25	c	601	CLA	O1D-CGD-O2D-CED
24	1	311	CHL	C2A-CAA-CBA-CGA
24	S	602	CHL	C8-C10-C11-C12
24	5	305	CHL	C2A-CAA-CBA-CGA
24	s	403	CHL	C8-C10-C11-C12
25	C	611	CLA	CBA-CGA-O2A-C1
25	c	605	CLA	CBA-CGA-O2A-C1
24	G	306	CHL	C8-C10-C11-C12
24	N	305	CHL	C8-C10-C11-C12
24	u	305	CHL	C13-C15-C16-C17
25	B	611	CLA	C13-C15-C16-C17
25	a	603	CLA	C15-C16-C17-C18
30	a	612	LHG	C31-C32-C33-C34
33	d	411	LMG	C12-C13-C14-C15
30	Y	318	LHG	C23-C24-C25-C26
30	y	319	LHG	C23-C24-C25-C26
33	i	101	LMG	C28-C29-C30-C31
24	3	304	CHL	O1D-CGD-O2D-CED
25	C	601	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	y	314	CLA	CBD-CGD-O2D-CED
30	A	601	LHG	C11-C12-C13-C14
29	3	301	0UR	O57-C45-C46-C47
29	G	301	0UR	O57-C45-C46-C47
29	g	301	0UR	O57-C45-C46-C47
24	G	305	CHL	C13-C15-C16-C17
24	G	306	CHL	C5-C6-C7-C8
24	9	305	CHL	C5-C6-C7-C8
24	u	306	CHL	C5-C6-C7-C8
24	n	305	CHL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	y	306	CHL	C10-C11-C12-C13
24	p	306	CHL	C10-C11-C12-C13
24	q	304	CHL	C8-C10-C11-C12
25	C	604	CLA	C13-C15-C16-C17
25	C	604	CLA	C15-C16-C17-C18
25	D	405	CLA	C5-C6-C7-C8
25	D	405	CLA	C15-C16-C17-C18
25	b	609	CLA	C8-C10-C11-C12
25	b	609	CLA	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
25	c	604	CLA	C13-C15-C16-C17
25	c	604	CLA	C15-C16-C17-C18
25	d	405	CLA	C15-C16-C17-C18
39	d	406	PL9	C47-C48-C49-C50
24	R	608	CHL	O1D-CGD-O2D-CED
24	r	309	CHL	O1D-CGD-O2D-CED
25	A	610	CLA	O1D-CGD-O2D-CED
30	Y	318	LHG	C7-C8-C9-C10
30	p	319	LHG	C23-C24-C25-C26
33	i	101	LMG	C10-C11-C12-C13
33	D	411	LMG	C18-C19-C20-C21
24	g	309	CHL	CBD-CGD-O2D-CED
25	1	315	CLA	O1D-CGD-O2D-CED
24	G	305	CHL	C8-C10-C11-C12
24	9	304	CHL	C15-C16-C17-C18
24	p	305	CHL	C8-C10-C11-C12
24	p	306	CHL	C5-C6-C7-C8
24	p	306	CHL	C8-C10-C11-C12
24	7	306	CHL	C5-C6-C7-C8
25	b	612	CLA	C5-C6-C7-C8
25	c	611	CLA	CBA-CGA-O2A-C1
33	D	401	LMG	C35-C36-C37-C38
25	B	613	CLA	O1D-CGD-O2D-CED
25	a	603	CLA	O1D-CGD-O2D-CED
24	8	304	CHL	C8-C10-C11-C12
24	y	305	CHL	C13-C15-C16-C17
24	7	305	CHL	C8-C10-C11-C12
25	B	608	CLA	C5-C6-C7-C8
25	a	603	CLA	C13-C15-C16-C17
25	n	315	CLA	O1D-CGD-O2D-CED
30	y	319	LHG	C7-C8-C9-C10
30	7	319	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	609	SQD	C7-C8-C9-C10
32	a	609	SQD	C23-C24-C25-C26
33	C	618	LMG	C28-C29-C30-C31
24	r	306	CHL	CBD-CGD-O2D-CED
25	3	316	CLA	CBD-CGD-O2D-CED
24	2	305	CHL	C2A-CAA-CBA-CGA
24	4	311	CHL	C2A-CAA-CBA-CGA
25	8	314	CLA	C2A-CAA-CBA-CGA
33	D	401	LMG	C11-C12-C13-C14
30	a	601	LHG	C11-C12-C13-C14
24	7	305	CHL	C13-C15-C16-C17
25	B	607	CLA	C8-C10-C11-C12
25	B	612	CLA	C5-C6-C7-C8
24	2	305	CHL	O1D-CGD-O2D-CED
24	5	305	CHL	O1D-CGD-O2D-CED
24	s	403	CHL	O1D-CGD-O2D-CED
24	G	306	CHL	C11-C10-C8-C7
24	u	305	CHL	C12-C13-C15-C16
24	p	306	CHL	C11-C12-C13-C15
24	7	306	CHL	C11-C12-C13-C15
25	8	312	CLA	C11-C10-C8-C7
25	y	315	CLA	C11-C10-C8-C7
25	q	313	CLA	C11-C10-C8-C7
24	G	311	CHL	O1A-CGA-O2A-C1
24	N	305	CHL	O1A-CGA-O2A-C1
24	Y	310	CHL	O1A-CGA-O2A-C1
24	u	306	CHL	O1A-CGA-O2A-C1
25	Y	314	CLA	O1A-CGA-O2A-C1
25	C	605	CLA	O1A-CGA-O2A-C1
25	c	605	CLA	O1A-CGA-O2A-C1
30	d	407	LHG	O10-C23-O8-C6
33	w	201	LMG	O10-C28-O8-C9
31	V	401	8CT	C16-C17-C18-C19
31	A	608	8CT	C12-C13-C14-C15
31	C	614	8CT	C18-C19-C20-C21
31	v	401	8CT	C16-C17-C18-C19
31	v	401	8CT	C18-C19-C20-C21
31	a	608	8CT	C12-C13-C14-C15
31	c	614	8CT	C18-C19-C20-C21
24	2	311	CHL	C2A-CAA-CBA-CGA
24	p	310	CHL	C2A-CAA-CBA-CGA
24	7	310	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	N	307	CLA	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
24	1	310	CHL	O1D-CGD-O2D-CED
24	2	306	CHL	O1D-CGD-O2D-CED
24	5	309	CHL	O1D-CGD-O2D-CED
25	G	317	CLA	O1D-CGD-O2D-CED
25	A	603	CLA	O1D-CGD-O2D-CED
25	s	410	CLA	O1D-CGD-O2D-CED
24	G	313	CHL	C8-C10-C11-C12
24	g	305	CHL	C8-C10-C11-C12
24	g	313	CHL	C8-C10-C11-C12
24	y	313	CHL	C5-C6-C7-C8
24	p	305	CHL	C13-C15-C16-C17
25	B	605	CLA	C5-C6-C7-C8
25	B	613	CLA	C10-C11-C12-C13
25	A	603	CLA	C13-C15-C16-C17
25	b	604	CLA	C5-C6-C7-C8
25	b	605	CLA	C5-C6-C7-C8
25	b	607	CLA	C8-C10-C11-C12
25	b	608	CLA	C5-C6-C7-C8
24	R	602	CHL	CBA-CGA-O2A-C1
24	r	303	CHL	CBA-CGA-O2A-C1
24	9	305	CHL	O1A-CGA-O2A-C1
25	D	405	CLA	O1A-CGA-O2A-C1
25	y	308	CLA	O1A-CGA-O2A-C1
25	y	315	CLA	O1A-CGA-O2A-C1
25	d	405	CLA	O1A-CGA-O2A-C1
33	W	201	LMG	O10-C28-O8-C9
25	b	602	CLA	CBD-CGD-O2D-CED
33	d	411	LMG	O6-C1-O1-C7
37	C	619	DGD	O6E-C1E-O5D-C6D
25	b	613	CLA	C10-C11-C12-C13
25	c	610	CLA	C15-C16-C17-C18
24	u	306	CHL	O1D-CGD-O2D-CED
24	y	313	CHL	O1D-CGD-O2D-CED
25	s	417	CLA	O1D-CGD-O2D-CED
24	9	305	CHL	O1D-CGD-O2D-CED
30	A	601	LHG	O2-C2-C3-O3
30	D	408	LHG	O2-C2-C3-O3
30	a	601	LHG	O2-C2-C3-O3
25	C	609	CLA	C3-C5-C6-C7
25	c	609	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	3	311	CHL	C2A-CAA-CBA-CGA
24	6	311	CHL	C2A-CAA-CBA-CGA
24	Y	304	CHL	C15-C16-C17-C18
24	u	305	CHL	C15-C16-C17-C18
24	p	305	CHL	C15-C16-C17-C18
24	7	305	CHL	C15-C16-C17-C18
25	B	609	CLA	C15-C16-C17-C18
25	d	405	CLA	C5-C6-C7-C8
25	B	604	CLA	CBA-CGA-O2A-C1
24	5	306	CHL	O1D-CGD-O2D-CED
24	n	305	CHL	O1D-CGD-O2D-CED
25	Y	307	CLA	O1A-CGA-O2A-C1
30	D	407	LHG	O10-C23-O8-C6
24	g	310	CHL	CBA-CGA-O2A-C1
24	9	305	CHL	C13-C15-C16-C17
24	g	306	CHL	C13-C15-C16-C17
25	B	604	CLA	C5-C6-C7-C8
25	b	609	CLA	C5-C6-C7-C8
24	G	306	CHL	O1D-CGD-O2D-CED
24	s	402	CHL	O1D-CGD-O2D-CED
29	8	301	0UR	O57-C45-C46-C47
29	n	301	0UR	O57-C45-C46-C47
29	q	301	0UR	O57-C45-C46-C47
24	1	304	CHL	CBD-CGD-O2D-CED
25	C	611	CLA	O1A-CGA-O2A-C1
37	C	620	DGD	C3A-C4A-C5A-C6A
24	u	306	CHL	C13-C15-C16-C17
25	B	609	CLA	C5-C6-C7-C8
25	A	603	CLA	C15-C16-C17-C18
25	C	610	CLA	C15-C16-C17-C18
30	1	318	LHG	C3-O3-P-O6
30	1	318	LHG	C4-O6-P-O3
30	2	319	LHG	C3-O3-P-O6
30	G	319	LHG	C3-O3-P-O6
30	G	319	LHG	C4-O6-P-O3
30	A	601	LHG	C3-O3-P-O6
30	C	617	LHG	C4-O6-P-O3
30	D	407	LHG	C4-O6-P-O3
30	D	408	LHG	C3-O3-P-O6
30	4	318	LHG	C4-O6-P-O3
30	5	319	LHG	C3-O3-P-O6
30	g	319	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	g	319	LHG	C4-O6-P-O3
30	p	319	LHG	C3-O3-P-O6
30	a	601	LHG	C3-O3-P-O6
30	c	617	LHG	C4-O6-P-O3
30	d	407	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O3
30	7	319	LHG	C3-O3-P-O6
24	Y	304	CHL	C3-C5-C6-C7
24	y	305	CHL	C3-C5-C6-C7
24	8	310	CHL	CBA-CGA-O2A-C1
24	n	305	CHL	CBA-CGA-O2A-C1
24	q	311	CHL	CBA-CGA-O2A-C1
24	y	310	CHL	O1D-CGD-O2D-CED
24	n	309	CHL	CBD-CGD-O2D-CED
33	D	411	LMG	C29-C30-C31-C32
24	G	306	CHL	C10-C11-C12-C13
24	S	602	CHL	O1D-CGD-O2D-CED
24	Y	309	CHL	O1D-CGD-O2D-CED
24	4	310	CHL	O1D-CGD-O2D-CED
24	4	312	CHL	O1D-CGD-O2D-CED
25	8	312	CLA	O1D-CGD-O2D-CED
25	4	315	CLA	O1D-CGD-O2D-CED
25	y	308	CLA	O1D-CGD-O2D-CED
24	N	304	CHL	C4-C3-C5-C6
24	n	304	CHL	C4-C3-C5-C6
29	N	301	0UR	O57-C45-C46-C47
24	N	304	CHL	O1D-CGD-O2D-CED
25	R	613	CLA	O1D-CGD-O2D-CED
33	d	401	LMG	C35-C36-C37-C38
24	3	309	CHL	C2A-CAA-CBA-CGA
24	S	602	CHL	C2A-CAA-CBA-CGA
24	G	306	CHL	C2A-CAA-CBA-CGA
24	9	311	CHL	C2A-CAA-CBA-CGA
24	N	309	CHL	C2A-CAA-CBA-CGA
24	Y	305	CHL	C2A-CAA-CBA-CGA
24	8	309	CHL	C2A-CAA-CBA-CGA
24	5	311	CHL	C2A-CAA-CBA-CGA
24	6	310	CHL	C2A-CAA-CBA-CGA
24	g	306	CHL	C2A-CAA-CBA-CGA
24	n	305	CHL	C2A-CAA-CBA-CGA
24	y	306	CHL	C2A-CAA-CBA-CGA
24	p	306	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	s	403	CHL	C2A-CAA-CBA-CGA
24	7	306	CHL	C2A-CAA-CBA-CGA
24	G	313	CHL	C16-C17-C18-C20
24	Y	312	CHL	C16-C17-C18-C19
24	y	313	CHL	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
25	C	610	CLA	C3-C5-C6-C7
24	Y	312	CHL	O1D-CGD-O2D-CED
24	y	311	CHL	CBA-CGA-O2A-C1
25	b	604	CLA	CBA-CGA-O2A-C1
25	A	604	CLA	C13-C15-C16-C17
25	a	607	CLA	C8-C10-C11-C12
33	D	411	LMG	C20-C21-C22-C23
37	C	619	DGD	O6D-C5D-C6D-O5D
24	g	306	CHL	O1D-CGD-O2D-CED
24	n	304	CHL	O1D-CGD-O2D-CED
25	9	307	CLA	O1D-CGD-O2D-CED
31	V	401	8CT	C18-C19-C20-C21
31	T	101	8CT	C12-C13-C14-C15
31	B	617	8CT	C18-C19-C20-C21
31	C	615	8CT	C18-C19-C20-C21
31	t	101	8CT	C12-C13-C14-C15
31	b	617	8CT	C18-C19-C20-C21
31	c	615	8CT	C18-C19-C20-C21
30	D	407	LHG	C7-C8-C9-C10
24	S	601	CHL	O1D-CGD-O2D-CED
25	S	609	CLA	O1D-CGD-O2D-CED
25	2	315	CLA	CBD-CGD-O2D-CED
32	A	609	SQD	C8-C7-O47-C45
33	m	101	LMG	C11-C10-O7-C8
24	g	306	CHL	C10-C11-C12-C13
24	y	313	CHL	C8-C10-C11-C12
24	7	306	CHL	C8-C10-C11-C12
37	c	618	DGD	O6D-C5D-C6D-O5D
25	y	317	CLA	C6-C7-C8-C10
30	9	318	LHG	C14-C15-C16-C17
30	N	318	LHG	C14-C15-C16-C17
30	Y	318	LHG	C15-C16-C17-C18
30	A	601	LHG	C15-C16-C17-C18
30	y	319	LHG	C14-C15-C16-C17
30	a	601	LHG	C15-C16-C17-C18
32	a	609	SQD	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	609	SQD	C12-C13-C14-C15
33	D	411	LMG	C30-C31-C32-C33
24	1	312	CHL	O1D-CGD-O2D-CED
24	2	309	CHL	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	D	405	CLA	O1D-CGD-O2D-CED
24	g	313	CHL	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
37	c	618	DGD	C2A-C1A-O1G-C1G
30	2	319	LHG	C27-C28-C29-C30
30	5	319	LHG	C27-C28-C29-C30
30	p	319	LHG	C30-C31-C32-C33
30	7	319	LHG	C30-C31-C32-C33
32	B	618	SQD	C33-C34-C35-C36
32	b	618	SQD	C9-C10-C11-C12
32	b	618	SQD	C33-C34-C35-C36
32	D	409	SQD	C44-C45-O47-C7
32	d	409	SQD	C44-C45-O47-C7
24	1	309	CHL	O1D-CGD-O2D-CED
24	Y	308	CHL	O1D-CGD-O2D-CED
24	g	313	CHL	O1D-CGD-O2D-CED
25	C	602	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	c	602	CLA	O1D-CGD-O2D-CED
33	m	101	LMG	O9-C10-O7-C8
24	R	601	CHL	CBD-CGD-O2D-CED
24	p	310	CHL	CBD-CGD-O2D-CED
32	b	618	SQD	C11-C12-C13-C14
24	g	318	CHL	O1D-CGD-O2D-CED
24	y	309	CHL	O1D-CGD-O2D-CED
24	p	305	CHL	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
30	4	318	LHG	C5-C4-O6-P
25	Y	316	CLA	C6-C7-C8-C10
30	g	319	LHG	C26-C27-C28-C29
30	p	319	LHG	C12-C13-C14-C15
32	B	618	SQD	C9-C10-C11-C12
33	d	411	LMG	C16-C17-C18-C19
24	3	305	CHL	O1D-CGD-O2D-CED
24	8	304	CHL	O1D-CGD-O2D-CED
24	6	305	CHL	O1D-CGD-O2D-CED
24	q	303	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	6	316	CLA	O1D-CGD-O2D-CED
24	Y	312	CHL	C8-C10-C11-C12
24	p	312	CHL	CBA-CGA-O2A-C1
24	7	312	CHL	CBA-CGA-O2A-C1
30	D	408	LHG	C9-C10-C11-C12
30	p	319	LHG	C28-C29-C30-C31
30	d	407	LHG	C30-C31-C32-C33
32	B	618	SQD	C11-C12-C13-C14
33	d	411	LMG	C17-C18-C19-C20
30	g	319	LHG	C23-C24-C25-C26
24	G	318	CHL	O1D-CGD-O2D-CED
26	9	303	0IE	C14-C15-C16-C17
32	D	409	SQD	C2-C1-O6-C44
32	d	409	SQD	C2-C1-O6-C44
33	C	618	LMG	C2-C1-O1-C7
33	i	101	LMG	C2-C1-O1-C7
33	d	411	LMG	C2-C1-O1-C7
37	C	619	DGD	C2E-C1E-O5D-C6D
37	c	618	DGD	C2E-C1E-O5D-C6D
24	p	306	CHL	CBA-CGA-O2A-C1
35	D	403	PHO	CBA-CGA-O2A-C1
35	d	403	PHO	CBA-CGA-O2A-C1
30	D	408	LHG	C25-C26-C27-C28
30	5	319	LHG	C26-C27-C28-C29
30	7	319	LHG	C28-C29-C30-C31
33	d	401	LMG	C17-C18-C19-C20
24	8	304	CHL	C5-C6-C7-C8
25	c	611	CLA	O1A-CGA-O2A-C1
24	9	304	CHL	C16-C17-C18-C19
24	9	304	CHL	C16-C17-C18-C20
24	Y	304	CHL	C16-C17-C18-C19
25	B	602	CLA	C16-C17-C18-C20
25	B	606	CLA	C16-C17-C18-C20
25	B	608	CLA	C6-C7-C8-C10
25	b	606	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C20
25	a	603	CLA	C16-C17-C18-C20
24	G	305	CHL	O1D-CGD-O2D-CED
24	6	308	CHL	O1D-CGD-O2D-CED
24	u	305	CHL	O1D-CGD-O2D-CED
24	q	304	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	610	CLA	O1D-CGD-O2D-CED
25	u	308	CLA	O1D-CGD-O2D-CED
25	d	405	CLA	O1D-CGD-O2D-CED
25	g	317	CLA	C6-C7-C8-C10
30	2	319	LHG	C26-C27-C28-C29
30	n	318	LHG	C14-C15-C16-C17
32	a	609	SQD	C9-C10-C11-C12
33	D	401	LMG	C37-C38-C39-C40
37	C	620	DGD	C2A-C3A-C4A-C5A
24	g	306	CHL	C6-C7-C8-C9
25	B	603	CLA	C14-C13-C15-C16
25	7	315	CLA	C6-C7-C8-C9
24	G	313	CHL	O1D-CGD-O2D-CED
24	5	310	CHL	O1D-CGD-O2D-CED
25	q	315	CLA	C2A-CAA-CBA-CGA
30	y	319	LHG	C15-C16-C17-C18
32	B	618	SQD	C12-C13-C14-C15
33	D	401	LMG	C17-C18-C19-C20
37	C	620	DGD	CCB-CDB-CEB-CFB
25	A	607	CLA	C8-C10-C11-C12
24	G	310	CHL	CBA-CGA-O2A-C1
24	G	310	CHL	C2A-CAA-CBA-CGA
24	g	305	CHL	C2A-CAA-CBA-CGA
28	S	617	NEX	C31-C32-C33-C40
28	9	319	NEX	C31-C32-C33-C40
28	5	304	NEX	C31-C32-C33-C40
28	u	304	NEX	C31-C32-C33-C40
28	p	304	NEX	C31-C32-C33-C40
31	S	615	8CT	C27-C26-C28-C29
31	B	617	8CT	C10-C11-C12-C40
31	C	614	8CT	C14-C15-C16-C39
31	t	101	8CT	C14-C15-C16-C39
31	b	617	8CT	C10-C11-C12-C40
31	c	614	8CT	C14-C15-C16-C39
31	d	410	8CT	C10-C11-C12-C40
31	s	416	8CT	C27-C26-C28-C29
30	D	407	LHG	C15-C16-C17-C18
30	y	319	LHG	C27-C28-C29-C30
33	D	411	LMG	C35-C36-C37-C38
30	2	319	LHG	O1-C1-C2-C3
30	9	318	LHG	O1-C1-C2-C3
30	N	318	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	617	LHG	O1-C1-C2-C3
30	n	318	LHG	O1-C1-C2-C3
30	c	617	LHG	O1-C1-C2-C3
30	d	408	LHG	O1-C1-C2-C3
29	8	301	0UR	C5-C6-C7-C8
29	4	301	0UR	C5-C6-C7-C8
29	6	301	0UR	C5-C6-C7-C8
29	n	301	0UR	C5-C6-C7-C8
31	S	615	8CT	C25-C26-C28-C29
31	B	617	8CT	C10-C11-C12-C13
31	C	614	8CT	C14-C15-C16-C17
31	c	614	8CT	C14-C15-C16-C17
31	d	410	8CT	C10-C11-C12-C13
31	s	416	8CT	C25-C26-C28-C29
25	y	317	CLA	C3-C5-C6-C7
35	D	403	PHO	C3-C5-C6-C7
35	d	403	PHO	C3-C5-C6-C7
24	G	306	CHL	C13-C15-C16-C17
24	Y	312	CHL	C5-C6-C7-C8
24	u	305	CHL	C8-C10-C11-C12
24	q	304	CHL	C5-C6-C7-C8
30	Y	318	LHG	C27-C28-C29-C30
30	d	407	LHG	C15-C16-C17-C18
37	c	619	DGD	CCB-CDB-CEB-CFB
29	Y	301	0UR	O44-C45-C46-C47
29	y	301	0UR	O44-C45-C46-C47
24	q	309	CHL	CBA-CGA-O2A-C1
30	d	407	LHG	C7-C8-C9-C10
33	w	201	LMG	C10-C11-C12-C13
24	2	310	CHL	O1D-CGD-O2D-CED
24	4	309	CHL	O1D-CGD-O2D-CED
24	g	305	CHL	O1D-CGD-O2D-CED
25	r	314	CLA	O1D-CGD-O2D-CED
39	D	406	PL9	C47-C48-C49-C50
30	9	318	LHG	C15-C16-C17-C18
30	p	319	LHG	C14-C15-C16-C17
32	b	618	SQD	C12-C13-C14-C15
32	a	609	SQD	C11-C12-C13-C14
32	a	609	SQD	C13-C14-C15-C16
33	D	411	LMG	C34-C35-C36-C37
33	d	401	LMG	C37-C38-C39-C40
37	C	620	DGD	C8B-C9B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	R	605	CHL	C4B-C3B-CAB-CBB
24	r	306	CHL	C4B-C3B-CAB-CBB
25	Y	306	CLA	C4B-C3B-CAB-CBB
25	u	316	CLA	C4B-C3B-CAB-CBB
25	y	307	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB
24	G	305	CHL	C16-C17-C18-C19
24	G	305	CHL	C16-C17-C18-C20
24	G	313	CHL	C16-C17-C18-C19
24	Y	304	CHL	C16-C17-C18-C20
24	Y	312	CHL	C16-C17-C18-C20
24	g	305	CHL	C16-C17-C18-C19
24	g	305	CHL	C16-C17-C18-C20
24	g	313	CHL	C16-C17-C18-C19
24	u	305	CHL	C16-C17-C18-C20
24	p	305	CHL	C16-C17-C18-C19
24	p	305	CHL	C16-C17-C18-C20
24	7	305	CHL	C16-C17-C18-C19
24	7	305	CHL	C16-C17-C18-C20
25	B	602	CLA	C16-C17-C18-C19
25	A	603	CLA	C16-C17-C18-C20
25	C	602	CLA	C16-C17-C18-C19
25	C	604	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C20
25	c	604	CLA	C16-C17-C18-C19
25	c	604	CLA	C16-C17-C18-C20
32	D	409	SQD	O5-C1-O6-C44
32	d	409	SQD	O5-C1-O6-C44
33	i	101	LMG	O6-C1-O1-C7
37	c	618	DGD	O6E-C1E-O5D-C6D
24	9	304	CHL	C8-C10-C11-C12
24	y	306	CHL	C13-C15-C16-C17
25	C	602	CLA	C5-C6-C7-C8
24	s	406	CHL	O1D-CGD-O2D-CED
30	G	319	LHG	C26-C27-C28-C29
32	A	609	SQD	C9-C10-C11-C12
37	c	618	DGD	C4D-C5D-C6D-O5D
24	8	303	CHL	O1D-CGD-O2D-CED
25	2	308	CLA	O1D-CGD-O2D-CED
33	D	401	LMG	C15-C16-C17-C18
37	C	619	DGD	C3B-C4B-C5B-C6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	c	618	DGD	C3B-C4B-C5B-C6B
37	c	619	DGD	C9B-CAB-CBB-CCB
30	G	319	LHG	C23-C24-C25-C26
24	G	313	CHL	C13-C15-C16-C17
33	B	619	LMG	C17-C18-C19-C20
33	m	101	LMG	C18-C19-C20-C21
24	3	309	CHL	O1D-CGD-O2D-CED
24	6	312	CHL	O1D-CGD-O2D-CED
24	Y	319	CHL	CBA-CGA-O2A-C1
24	N	310	CHL	O1D-CGD-O2D-CED
24	Y	304	CHL	O1D-CGD-O2D-CED
24	r	307	CHL	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	r	304	CLA	O1D-CGD-O2D-CED
24	R	606	CHL	C3A-C2A-CAA-CBA
24	3	310	CHL	C3A-C2A-CAA-CBA
24	S	606	CHL	C3A-C2A-CAA-CBA
24	G	311	CHL	C3A-C2A-CAA-CBA
24	N	310	CHL	C3A-C2A-CAA-CBA
24	Y	310	CHL	C3A-C2A-CAA-CBA
24	Y	319	CHL	C3A-C2A-CAA-CBA
24	6	310	CHL	C3A-C2A-CAA-CBA
24	g	311	CHL	C3A-C2A-CAA-CBA
24	u	310	CHL	C3A-C2A-CAA-CBA
24	u	311	CHL	C3A-C2A-CAA-CBA
24	n	310	CHL	C3A-C2A-CAA-CBA
24	y	311	CHL	C3A-C2A-CAA-CBA
24	p	311	CHL	C3A-C2A-CAA-CBA
24	q	309	CHL	C3A-C2A-CAA-CBA
24	s	407	CHL	C3A-C2A-CAA-CBA
24	r	307	CHL	C3A-C2A-CAA-CBA
24	7	311	CHL	C3A-C2A-CAA-CBA
25	S	616	CLA	C3A-C2A-CAA-CBA
25	A	603	CLA	C3A-C2A-CAA-CBA
25	D	404	CLA	C3A-C2A-CAA-CBA
25	a	603	CLA	C3A-C2A-CAA-CBA
25	s	417	CLA	C3A-C2A-CAA-CBA
25	C	604	CLA	C5-C6-C7-C8
25	C	610	CLA	C10-C11-C12-C13
25	c	604	CLA	C5-C6-C7-C8
24	S	605	CHL	O1D-CGD-O2D-CED
25	c	604	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	s	411	CLA	O1D-CGD-O2D-CED
24	n	305	CHL	O1A-CGA-O2A-C1
24	y	311	CHL	O1A-CGA-O2A-C1
24	u	305	CHL	C16-C17-C18-C19
24	y	313	CHL	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C20
25	C	604	CLA	C16-C17-C18-C19
30	2	319	LHG	C28-C29-C30-C31
30	9	318	LHG	C26-C27-C28-C29
30	5	319	LHG	C28-C29-C30-C31
30	n	318	LHG	C12-C13-C14-C15
30	a	601	LHG	C13-C14-C15-C16
25	c	602	CLA	C5-C6-C7-C8
24	R	605	CHL	O1D-CGD-O2D-CED
25	5	308	CLA	O1D-CGD-O2D-CED
30	A	601	LHG	C4-C5-C6-O8
30	a	601	LHG	C4-C5-C6-O8
24	9	309	CHL	CBD-CGD-O2D-CED
25	G	308	CLA	CBD-CGD-O2D-CED
25	G	317	CLA	C6-C7-C8-C10
32	b	618	SQD	C14-C15-C16-C17
29	Y	301	0UR	O57-C45-C46-C47
29	y	301	0UR	O57-C45-C46-C47
24	8	310	CHL	O1A-CGA-O2A-C1
24	7	306	CHL	CBA-CGA-O2A-C1
35	a	606	PHO	CBA-CGA-O2A-C1
24	G	313	CHL	C2-C3-C5-C6
24	N	312	CHL	C2-C3-C5-C6
24	g	313	CHL	C2-C3-C5-C6
24	n	312	CHL	C2-C3-C5-C6
39	D	406	PL9	C12-C11-C9-C8
39	D	406	PL9	C43-C44-C46-C47
30	D	408	LHG	C8-C7-O7-C5
30	d	408	LHG	C8-C7-O7-C5
24	R	606	CHL	O1D-CGD-O2D-CED
25	b	604	CLA	O1D-CGD-O2D-CED
24	G	310	CHL	CBD-CGD-O2D-CED
25	S	612	CLA	C6-C7-C8-C10
30	9	318	LHG	C12-C13-C14-C15
30	9	318	LHG	C29-C30-C31-C32
25	B	606	CLA	C2A-CAA-CBA-CGA
25	n	307	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C2A-CAA-CBA-CGA
30	G	319	LHG	O1-C1-C2-O2
30	n	318	LHG	O1-C1-C2-O2
30	p	319	LHG	O1-C1-C2-O2
25	a	604	CLA	C13-C15-C16-C17
25	s	413	CLA	C6-C7-C8-C10
30	y	319	LHG	C11-C12-C13-C14
30	d	407	LHG	C31-C32-C33-C34
33	i	101	LMG	C37-C38-C39-C40
24	q	311	CHL	O1A-CGA-O2A-C1
25	B	604	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	C16-C17-C18-C19
24	R	605	CHL	C2B-C3B-CAB-CBB
24	r	306	CHL	C2B-C3B-CAB-CBB
25	S	604	CLA	C2B-C3B-CAB-CBB
25	9	316	CLA	C2B-C3B-CAB-CBB
25	B	607	CLA	C2B-C3B-CAB-CBB
25	u	316	CLA	C2B-C3B-CAB-CBB
25	y	307	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
25	b	607	CLA	C2B-C3B-CAB-CBB
30	1	318	LHG	O2-C2-C3-O3
37	C	620	DGD	C9B-CAB-CBB-CCB
24	9	311	CHL	CBA-CGA-O2A-C1
30	a	612	LHG	C12-C13-C14-C15
32	B	618	SQD	C14-C15-C16-C17
30	a	601	LHG	C7-C8-C9-C10
33	d	411	LMG	C10-C11-C12-C13
24	p	318	CHL	CBD-CGD-O2D-CED
25	C	612	CLA	CBD-CGD-O2D-CED
30	1	318	LHG	C28-C29-C30-C31
30	4	318	LHG	C28-C29-C30-C31
33	B	619	LMG	C18-C19-C20-C21
30	D	408	LHG	O9-C7-O7-C5
30	A	612	LHG	C12-C13-C14-C15
30	p	319	LHG	C10-C11-C12-C13
37	c	619	DGD	C3A-C4A-C5A-C6A
24	g	313	CHL	C13-C15-C16-C17
25	c	610	CLA	C10-C11-C12-C13
24	Y	319	CHL	O1A-CGA-O2A-C1
24	p	306	CHL	O1A-CGA-O2A-C1
24	q	309	CHL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	604	CLA	O1A-CGA-O2A-C1
35	d	403	PHO	O1A-CGA-O2A-C1
37	c	618	DGD	O1A-C1A-O1G-C1G
30	p	319	LHG	C25-C26-C27-C28
32	A	609	SQD	C11-C12-C13-C14
33	d	401	LMG	C15-C16-C17-C18
25	B	606	CLA	C16-C17-C18-C19
32	A	609	SQD	C7-C8-C9-C10
24	r	302	CHL	CBD-CGD-O2D-CED
31	S	614	8CT	C02-C03-C10-C11
31	S	615	8CT	C04-C03-C10-C11
31	X	601	8CT	C02-C03-C10-C11
31	T	101	8CT	C02-C03-C10-C11
31	A	608	8CT	C02-C03-C10-C11
31	C	613	8CT	C02-C03-C10-C11
31	C	614	8CT	C02-C03-C10-C11
31	C	615	8CT	C02-C03-C10-C11
31	D	410	8CT	C04-C03-C10-C11
31	x	601	8CT	C02-C03-C10-C11
31	t	101	8CT	C02-C03-C10-C11
31	a	608	8CT	C02-C03-C10-C11
31	c	613	8CT	C02-C03-C10-C11
31	c	614	8CT	C02-C03-C10-C11
31	c	615	8CT	C02-C03-C10-C11
31	d	410	8CT	C04-C03-C10-C11
31	s	415	8CT	C02-C03-C10-C11
31	s	416	8CT	C04-C03-C10-C11
32	a	609	SQD	C24-C25-C26-C27
33	D	411	LMG	C32-C33-C34-C35
37	C	620	DGD	CDB-CEB-CFB-CGB
25	C	604	CLA	O1D-CGD-O2D-CED
24	Y	305	CHL	CBA-CGA-O2A-C1
24	g	306	CHL	CBA-CGA-O2A-C1
25	B	608	CLA	CBA-CGA-O2A-C1
25	u	317	CLA	CBA-CGA-O2A-C1
25	b	608	CLA	CBA-CGA-O2A-C1
35	A	606	PHO	CBA-CGA-O2A-C1
25	D	405	CLA	C13-C15-C16-C17
25	d	405	CLA	C13-C15-C16-C17
33	w	201	LMG	C11-C10-O7-C8
25	n	306	CLA	O1D-CGD-O2D-CED
35	D	403	PHO	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	2	319	LHG	C14-C15-C16-C17
24	n	305	CHL	C5-C6-C7-C8
24	p	306	CHL	C13-C15-C16-C17
25	Y	313	CLA	O1D-CGD-O2D-CED
30	d	408	LHG	C31-C32-C33-C34
37	c	619	DGD	CDB-CEB-CFB-CGB
24	N	312	CHL	C4-C3-C5-C6
25	C	607	CLA	C4-C3-C5-C6
25	c	607	CLA	C4-C3-C5-C6
25	B	604	CLA	O1D-CGD-O2D-CED
24	G	305	CHL	C6-C7-C8-C10
24	G	306	CHL	C11-C12-C13-C15
24	9	304	CHL	C12-C13-C15-C16
24	Y	312	CHL	C11-C12-C13-C15
24	g	305	CHL	C6-C7-C8-C10
24	g	306	CHL	C11-C10-C8-C7
24	g	306	CHL	C11-C12-C13-C15
24	y	313	CHL	C11-C12-C13-C15
24	p	305	CHL	C12-C13-C15-C16
25	G	315	CLA	C6-C7-C8-C10
25	Y	314	CLA	C11-C10-C8-C7
25	B	603	CLA	C12-C13-C15-C16
25	B	606	CLA	C12-C13-C15-C16
25	C	603	CLA	C12-C13-C15-C16
25	C	604	CLA	C6-C7-C8-C10
25	g	315	CLA	C6-C7-C8-C10
25	p	315	CLA	C12-C13-C15-C16
25	b	606	CLA	C12-C13-C15-C16
25	c	603	CLA	C12-C13-C15-C16
25	c	604	CLA	C6-C7-C8-C10
25	7	315	CLA	C12-C13-C15-C16
39	d	406	PL9	C43-C44-C46-C47
25	Y	316	CLA	C3-C5-C6-C7
25	B	607	CLA	C3-C5-C6-C7
24	7	306	CHL	O1A-CGA-O2A-C1
35	a	606	PHO	O1A-CGA-O2A-C1
30	A	612	LHG	C11-C12-C13-C14
24	Y	304	CHL	C8-C10-C11-C12
30	d	408	LHG	O9-C7-O7-C5
37	C	619	DGD	O1B-C1B-O2G-C2G
37	c	618	DGD	O1B-C1B-O2G-C2G
37	C	620	DGD	C1B-C2B-C3B-C4B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	y	306	CHL	CBA-CGA-O2A-C1
37	C	619	DGD	C2A-C1A-O1G-C1G
24	G	305	CHL	C2A-CAA-CBA-CGA
24	8	304	CHL	C2A-CAA-CBA-CGA
24	q	304	CHL	C2A-CAA-CBA-CGA
25	3	316	CLA	C2A-CAA-CBA-CGA
25	9	307	CLA	C2A-CAA-CBA-CGA
25	8	312	CLA	C5-C6-C7-C8
32	b	618	SQD	C10-C11-C12-C13
25	N	316	CLA	C2A-CAA-CBA-CGA
25	n	316	CLA	C2A-CAA-CBA-CGA
25	5	315	CLA	CBD-CGD-O2D-CED
30	G	319	LHG	C14-C15-C16-C17
30	g	319	LHG	C27-C28-C29-C30
32	B	618	SQD	C10-C11-C12-C13
30	c	617	LHG	C9-C10-C11-C12
33	i	101	LMG	C17-C18-C19-C20
37	c	619	DGD	C8B-C9B-CAB-CBB
24	u	311	CHL	O1D-CGD-O2D-CED
25	S	610	CLA	O1D-CGD-O2D-CED
30	N	318	LHG	C12-C13-C14-C15
30	y	319	LHG	C12-C13-C14-C15
30	d	408	LHG	C9-C10-C11-C12
33	m	101	LMG	C17-C18-C19-C20
24	G	309	CHL	CBD-CGD-O2D-CED
24	G	306	CHL	CBA-CGA-O2A-C1
25	c	603	CLA	C16-C17-C18-C20
24	9	310	CHL	O1D-CGD-O2D-CED
24	7	305	CHL	O1D-CGD-O2D-CED
30	G	319	LHG	C15-C16-C17-C18
30	g	319	LHG	C15-C16-C17-C18
30	7	319	LHG	C25-C26-C27-C28
33	B	619	LMG	C28-C29-C30-C31
32	a	609	SQD	C8-C7-O47-C45
33	B	619	LMG	C11-C10-O7-C8
37	C	619	DGD	C2B-C1B-O2G-C2G
37	c	618	DGD	C2B-C1B-O2G-C2G
24	u	309	CHL	O1D-CGD-O2D-CED
30	C	617	LHG	C9-C10-C11-C12
25	b	604	CLA	C8-C10-C11-C12
25	a	607	CLA	C5-C6-C7-C8
35	A	606	PHO	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	7	310	CHL	CBD-CGD-O2D-CED
35	A	606	PHO	O1A-CGA-O2A-C1
30	a	612	LHG	C11-C12-C13-C14
32	A	609	SQD	O49-C7-O47-C45
33	B	619	LMG	O9-C10-O7-C8
33	w	201	LMG	O9-C10-O7-C8
25	b	607	CLA	C3-C5-C6-C7
24	n	317	CHL	O1D-CGD-O2D-CED
24	y	305	CHL	C16-C17-C18-C20
25	a	603	CLA	C16-C17-C18-C19
30	A	601	LHG	C13-C14-C15-C16
33	d	411	LMG	C14-C15-C16-C17
24	g	313	CHL	C15-C16-C17-C18
24	7	306	CHL	C13-C15-C16-C17
25	A	607	CLA	C5-C6-C7-C8
35	a	606	PHO	C13-C15-C16-C17
24	G	313	CHL	C4-C3-C5-C6
24	g	313	CHL	C4-C3-C5-C6
24	n	312	CHL	C4-C3-C5-C6
24	u	312	CHL	CBA-CGA-O2A-C1
24	N	304	CHL	C2-C3-C5-C6
24	n	304	CHL	C2-C3-C5-C6
30	G	319	LHG	C28-C29-C30-C31
24	G	306	CHL	C11-C10-C8-C9
24	g	306	CHL	C11-C10-C8-C9
24	y	306	CHL	C11-C10-C8-C9
25	G	315	CLA	C6-C7-C8-C9
25	8	312	CLA	C6-C7-C8-C9
25	B	603	CLA	C6-C7-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	g	315	CLA	C6-C7-C8-C9
25	p	315	CLA	C14-C13-C15-C16
25	q	313	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	b	606	CLA	C14-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
25	c	607	CLA	C11-C10-C8-C9
25	c	611	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	7	315	CLA	C14-C13-C15-C16
24	N	305	CHL	C3-C5-C6-C7
24	7	306	CHL	C3-C5-C6-C7
24	n	310	CHL	O1D-CGD-O2D-CED
24	2	306	CHL	C2A-CAA-CBA-CGA
24	3	305	CHL	C2A-CAA-CBA-CGA
24	5	306	CHL	C2A-CAA-CBA-CGA
24	6	305	CHL	C2A-CAA-CBA-CGA
24	q	310	CHL	C2A-CAA-CBA-CGA
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
25	s	413	CLA	C2A-CAA-CBA-CGA
28	R	616	NEX	C31-C32-C33-C40
28	1	303	NEX	C31-C32-C33-C40
28	2	304	NEX	C31-C32-C33-C40
28	G	304	NEX	C31-C32-C33-C40
28	4	303	NEX	C31-C32-C33-C40
28	g	304	NEX	C31-C32-C33-C40
28	y	304	NEX	C31-C32-C33-C40
28	r	317	NEX	C31-C32-C33-C40
28	7	304	NEX	C31-C32-C33-C40
24	2	318	CHL	O1D-CGD-O2D-CED
24	n	312	CHL	O1D-CGD-O2D-CED
25	B	602	CLA	O1D-CGD-O2D-CED
30	y	319	LHG	C10-C11-C12-C13
31	B	617	8CT	C25-C26-C28-C29
31	b	617	8CT	C25-C26-C28-C29
24	Y	305	CHL	O1A-CGA-O2A-C1
24	g	306	CHL	O1A-CGA-O2A-C1
25	B	608	CLA	O1A-CGA-O2A-C1
25	u	317	CLA	O1A-CGA-O2A-C1
25	b	608	CLA	O1A-CGA-O2A-C1
24	R	606	CHL	C1A-C2A-CAA-CBA
24	1	305	CHL	C1A-C2A-CAA-CBA
24	3	310	CHL	C1A-C2A-CAA-CBA
24	S	606	CHL	C1A-C2A-CAA-CBA
24	G	311	CHL	C1A-C2A-CAA-CBA
24	N	310	CHL	C1A-C2A-CAA-CBA
24	Y	304	CHL	C1A-C2A-CAA-CBA
24	Y	305	CHL	C1A-C2A-CAA-CBA
24	Y	310	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Y	319	CHL	C1A-C2A-CAA-CBA
24	4	305	CHL	C1A-C2A-CAA-CBA
24	6	310	CHL	C1A-C2A-CAA-CBA
24	g	311	CHL	C1A-C2A-CAA-CBA
24	u	311	CHL	C1A-C2A-CAA-CBA
24	u	312	CHL	C1A-C2A-CAA-CBA
24	n	310	CHL	C1A-C2A-CAA-CBA
24	y	305	CHL	C1A-C2A-CAA-CBA
24	y	306	CHL	C1A-C2A-CAA-CBA
24	y	311	CHL	C1A-C2A-CAA-CBA
24	p	311	CHL	C1A-C2A-CAA-CBA
24	q	309	CHL	C1A-C2A-CAA-CBA
24	s	407	CHL	C1A-C2A-CAA-CBA
24	r	307	CHL	C1A-C2A-CAA-CBA
24	7	311	CHL	C1A-C2A-CAA-CBA
25	R	613	CLA	C1A-C2A-CAA-CBA
25	1	313	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C1A-C2A-CAA-CBA
25	N	313	CLA	C1A-C2A-CAA-CBA
25	A	603	CLA	C1A-C2A-CAA-CBA
25	4	313	CLA	C1A-C2A-CAA-CBA
25	n	313	CLA	C1A-C2A-CAA-CBA
25	a	603	CLA	C1A-C2A-CAA-CBA
25	s	410	CLA	C1A-C2A-CAA-CBA
25	r	313	CLA	C1A-C2A-CAA-CBA
25	r	314	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C6-C7-C8-C10
25	c	602	CLA	C16-C17-C18-C19
31	X	601	8CT	C23-C24-C25-C26
24	R	602	CHL	O1A-CGA-O2A-C1
24	g	310	CHL	O1A-CGA-O2A-C1
24	r	303	CHL	O1A-CGA-O2A-C1
25	C	610	CLA	C13-C15-C16-C17
30	d	408	LHG	C3-O3-P-O6
30	N	318	LHG	C23-C24-C25-C26
30	n	318	LHG	C23-C24-C25-C26
30	A	601	LHG	C5-C4-O6-P
24	9	308	CHL	O1D-CGD-O2D-CED
24	Y	305	CHL	C13-C15-C16-C17
24	g	306	CHL	C5-C6-C7-C8
25	q	313	CLA	C5-C6-C7-C8
25	7	315	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	9	318	LHG	O6-C4-C5-C6
24	3	308	CHL	O1D-CGD-O2D-CED
24	6	309	CHL	O1D-CGD-O2D-CED
24	y	305	CHL	O1D-CGD-O2D-CED
25	q	312	CLA	O1D-CGD-O2D-CED
30	a	601	LHG	C25-C26-C27-C28
25	D	404	CLA	C10-C11-C12-C13
25	A	603	CLA	C16-C17-C18-C19
24	3	312	CHL	O1D-CGD-O2D-CED
30	d	407	LHG	C14-C15-C16-C17
24	y	306	CHL	C8-C10-C11-C12
25	c	610	CLA	C13-C15-C16-C17
33	m	101	LMG	C10-C11-C12-C13
33	D	411	LMG	C15-C16-C17-C18
33	w	201	LMG	C18-C19-C20-C21
30	g	319	LHG	C12-C13-C14-C15
25	B	611	CLA	C10-C11-C12-C13
30	A	601	LHG	C25-C26-C27-C28
30	7	319	LHG	C10-C11-C12-C13
24	y	306	CHL	O1A-CGA-O2A-C1
37	C	619	DGD	O1A-C1A-O1G-C1G
25	c	604	CLA	C8-C10-C11-C12
25	B	603	CLA	C2A-CAA-CBA-CGA
25	N	306	CLA	O1D-CGD-O2D-CED
25	A	607	CLA	C3-C5-C6-C7
25	a	607	CLA	C3-C5-C6-C7
30	C	617	LHG	C4-C5-C6-O8
30	4	318	LHG	C4-C5-C6-O8
30	c	617	LHG	C4-C5-C6-O8
32	B	618	SQD	O6-C44-C45-C46
32	b	618	SQD	O6-C44-C45-C46
33	D	401	LMG	C7-C8-C9-O8
33	D	411	LMG	C7-C8-C9-O8
33	d	401	LMG	C7-C8-C9-O8
33	d	411	LMG	O1-C7-C8-C9
37	C	620	DGD	O1G-C1G-C2G-C3G
24	N	317	CHL	O1D-CGD-O2D-CED
25	B	612	CLA	C8-C10-C11-C12
25	C	607	CLA	C10-C11-C12-C13
24	G	306	CHL	C15-C16-C17-C18
30	y	319	LHG	C11-C10-C9-C8
24	9	304	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	N	312	CHL	O1D-CGD-O2D-CED
24	u	318	CHL	O1D-CGD-O2D-CED
33	D	411	LMG	C11-C12-C13-C14
33	W	201	LMG	C11-C12-C13-C14
25	y	314	CLA	O1D-CGD-O2D-CED
30	g	319	LHG	C14-C15-C16-C17
33	d	411	LMG	C21-C22-C23-C24
24	G	311	CHL	CAA-CBA-CGA-O2A
30	A	612	LHG	C23-C24-C25-C26
30	G	319	LHG	C27-C28-C29-C30
30	9	318	LHG	C10-C11-C12-C13
30	Y	318	LHG	C11-C10-C9-C8
37	c	619	DGD	C6A-C7A-C8A-C9A
33	m	101	LMG	O6-C1-O1-C7
25	b	611	CLA	C10-C11-C12-C13
24	S	608	CHL	C2C-C3C-CAC-CBC
30	D	407	LHG	C14-C15-C16-C17
30	1	318	LHG	O1-C1-C2-O2
30	D	407	LHG	O1-C1-C2-O2
30	4	318	LHG	O1-C1-C2-O2
30	g	319	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
30	7	319	LHG	O1-C1-C2-O2
30	C	617	LHG	C10-C11-C12-C13
30	c	617	LHG	C10-C11-C12-C13
24	G	306	CHL	O1A-CGA-O2A-C1
30	d	408	LHG	C7-C8-C9-C10
37	C	620	DGD	C6A-C7A-C8A-C9A
30	4	318	LHG	C15-C16-C17-C18
37	C	619	DGD	C8B-C9B-CAB-CBB
24	5	311	CHL	CBA-CGA-O2A-C1
24	5	318	CHL	O1D-CGD-O2D-CED
24	g	309	CHL	O1D-CGD-O2D-CED
24	y	313	CHL	C4-C3-C5-C6
24	q	304	CHL	C11-C12-C13-C14
30	g	319	LHG	C28-C29-C30-C31
24	4	304	CHL	O1D-CGD-O2D-CED
30	a	612	LHG	C23-C24-C25-C26
24	r	307	CHL	CBA-CGA-O2A-C1
25	9	316	CLA	CBA-CGA-O2A-C1
25	c	608	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2	313	CHL	CBD-CGD-O2D-CED
24	5	313	CHL	CBD-CGD-O2D-CED
24	G	313	CHL	C15-C16-C17-C18
25	c	602	CLA	C13-C15-C16-C17
25	c	607	CLA	C10-C11-C12-C13
30	1	318	LHG	C15-C16-C17-C18
30	Y	318	LHG	C26-C27-C28-C29
30	y	319	LHG	C17-C18-C19-C20
37	c	618	DGD	C8B-C9B-CAB-CBB
24	p	311	CHL	C2A-CAA-CBA-CGA
25	G	308	CLA	C2A-CAA-CBA-CGA
25	B	605	CLA	C13-C15-C16-C17
24	s	403	CHL	C2-C1-O2A-CGA
24	r	306	CHL	O1D-CGD-O2D-CED
25	N	314	CLA	C5-C6-C7-C8
25	p	315	CLA	C5-C6-C7-C8
25	b	612	CLA	C8-C10-C11-C12
24	g	306	CHL	C15-C16-C17-C18
25	s	413	CLA	C11-C10-C8-C7
30	Y	318	LHG	C10-C11-C12-C13
30	y	319	LHG	C26-C27-C28-C29
32	A	609	SQD	C14-C15-C16-C17
24	N	310	CHL	CBA-CGA-O2A-C1
24	8	304	CHL	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	C	608	CLA	CBA-CGA-O2A-C1
25	p	317	CLA	CBA-CGA-O2A-C1
30	A	612	LHG	O6-C4-C5-O7
30	p	319	LHG	O6-C4-C5-O7
30	7	319	LHG	O6-C4-C5-O7
24	y	305	CHL	C16-C17-C18-C19
25	C	603	CLA	C16-C17-C18-C20
30	D	407	LHG	C19-C20-C21-C22
24	Y	305	CHL	C8-C10-C11-C12
25	b	605	CLA	C13-C15-C16-C17
24	2	311	CHL	CBA-CGA-O2A-C1
25	3	316	CLA	O1D-CGD-O2D-CED
24	s	409	CHL	C2C-C3C-CAC-CBC
32	A	609	SQD	C12-C13-C14-C15
30	1	318	LHG	C23-C24-C25-C26
33	W	201	LMG	C10-C11-C12-C13
25	c	603	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	W	201	LMG	C2-C1-O1-C7
24	y	306	CHL	C15-C16-C17-C18
30	A	601	LHG	O7-C5-C6-O8
30	a	601	LHG	O7-C5-C6-O8
33	D	401	LMG	O7-C8-C9-O8
33	d	401	LMG	O7-C8-C9-O8
24	n	309	CHL	O1D-CGD-O2D-CED
25	S	612	CLA	C11-C10-C8-C7
30	1	318	LHG	C12-C13-C14-C15
30	G	319	LHG	C12-C13-C14-C15
33	w	201	LMG	C16-C17-C18-C19
25	C	601	CLA	C8-C10-C11-C12
25	7	315	CLA	C5-C6-C7-C8
24	Y	309	CHL	CBA-CGA-O2A-C1
24	8	304	CHL	C11-C12-C13-C14
30	D	408	LHG	C10-C11-C12-C13
30	D	408	LHG	C26-C27-C28-C29
25	c	610	CLA	C4-C3-C5-C6
39	d	406	PL9	C45-C44-C46-C47
25	B	606	CLA	C13-C15-C16-C17
25	C	611	CLA	C10-C11-C12-C13
24	9	305	CHL	C12-C13-C15-C16
24	N	305	CHL	C11-C10-C8-C7
24	Y	304	CHL	C12-C13-C15-C16
24	Y	305	CHL	C11-C12-C13-C15
24	Y	305	CHL	C12-C13-C15-C16
24	8	304	CHL	C6-C7-C8-C10
24	g	313	CHL	C12-C13-C15-C16
24	u	306	CHL	C12-C13-C15-C16
24	y	306	CHL	C11-C10-C8-C7
24	p	305	CHL	C11-C12-C13-C15
24	p	306	CHL	C6-C7-C8-C10
24	q	304	CHL	C6-C7-C8-C10
24	7	305	CHL	C11-C12-C13-C15
24	7	305	CHL	C12-C13-C15-C16
25	2	315	CLA	C6-C7-C8-C10
25	8	312	CLA	C6-C7-C8-C10
25	B	603	CLA	C6-C7-C8-C10
25	B	604	CLA	C12-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C15
25	B	611	CLA	C12-C13-C15-C16
25	A	604	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	601	CLA	C12-C13-C15-C16
25	D	404	CLA	C11-C10-C8-C7
25	q	313	CLA	C6-C7-C8-C10
25	b	603	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C6-C7-C8-C10
25	b	609	CLA	C12-C13-C15-C16
25	b	611	CLA	C12-C13-C15-C16
25	a	604	CLA	C12-C13-C15-C16
25	c	608	CLA	C11-C12-C13-C15
25	c	611	CLA	C11-C10-C8-C7
24	G	305	CHL	C11-C10-C8-C9
24	G	306	CHL	C14-C13-C15-C16
24	G	313	CHL	C6-C7-C8-C9
24	G	313	CHL	C11-C12-C13-C14
24	N	305	CHL	C11-C10-C8-C9
24	Y	304	CHL	C14-C13-C15-C16
24	Y	305	CHL	C11-C10-C8-C9
24	Y	305	CHL	C14-C13-C15-C16
24	g	306	CHL	C14-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	B	609	CLA	C14-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C9
25	C	607	CLA	C11-C10-C8-C9
25	C	611	CLA	C11-C10-C8-C9
25	C	611	CLA	C14-C13-C15-C16
25	D	404	CLA	C11-C10-C8-C9
25	5	315	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	604	CLA	C14-C13-C15-C16
25	b	609	CLA	C14-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C9
25	c	611	CLA	C11-C10-C8-C9
25	d	404	CLA	C11-C10-C8-C9
31	x	601	8CT	C23-C24-C25-C26
30	5	319	LHG	C23-C24-C25-C26
24	R	606	CHL	CBA-CGA-O2A-C1
24	n	310	CHL	CBA-CGA-O2A-C1
24	q	304	CHL	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	s	413	CLA	CBA-CGA-O2A-C1
25	7	317	CLA	CBA-CGA-O2A-C1
25	y	315	CLA	C5-C6-C7-C8
25	S	612	CLA	C2A-CAA-CBA-CGA
25	C	601	CLA	C2A-CAA-CBA-CGA
24	N	308	CHL	CBD-CGD-O2D-CED
29	1	301	0UR	C22-C16-C17-C18
29	3	301	0UR	C5-C6-C7-C20
29	4	301	0UR	C22-C16-C17-C18
31	C	615	8CT	C10-C11-C12-C40
25	b	609	CLA	C16-C17-C18-C20
29	1	301	0UR	C5-C6-C7-C8
29	4	301	0UR	C15-C16-C17-C18
29	q	301	0UR	C5-C6-C7-C8
31	C	615	8CT	C10-C11-C12-C13
31	D	410	8CT	C10-C11-C12-C13
24	Y	305	CHL	C15-C16-C17-C18
30	g	319	LHG	C10-C11-C12-C13
33	D	411	LMG	C36-C37-C38-C39
25	b	602	CLA	O1D-CGD-O2D-CED
25	C	604	CLA	C8-C10-C11-C12
33	W	201	LMG	C11-C10-O7-C8
30	G	319	LHG	C10-C11-C12-C13
30	d	407	LHG	C19-C20-C21-C22
25	S	612	CLA	CBA-CGA-O2A-C1
25	9	307	CLA	CBA-CGA-O2A-C1
24	9	305	CHL	C15-C16-C17-C18
25	p	317	CLA	C6-C7-C8-C10
30	D	407	LHG	C32-C33-C34-C35
33	C	618	LMG	C16-C17-C18-C19
24	y	313	CHL	C13-C15-C16-C17
25	B	603	CLA	C10-C11-C12-C13
25	B	604	CLA	C8-C10-C11-C12
25	p	315	CLA	C8-C10-C11-C12
25	b	615	CLA	C15-C16-C17-C18
24	p	312	CHL	O1A-CGA-O2A-C1
24	7	312	CHL	O1A-CGA-O2A-C1
24	7	318	CHL	CBD-CGD-O2D-CED
35	d	403	PHO	CBD-CGD-O2D-CED
24	u	306	CHL	C15-C16-C17-C18
30	n	318	LHG	C15-C16-C17-C18
25	R	604	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	1	314	CLA	C4B-C3B-CAB-CBB
25	2	307	CLA	C4B-C3B-CAB-CBB
25	S	604	CLA	C4B-C3B-CAB-CBB
25	S	616	CLA	C4B-C3B-CAB-CBB
25	9	315	CLA	C4B-C3B-CAB-CBB
25	B	607	CLA	C4B-C3B-CAB-CBB
25	4	314	CLA	C4B-C3B-CAB-CBB
25	5	307	CLA	C4B-C3B-CAB-CBB
25	u	315	CLA	C4B-C3B-CAB-CBB
25	p	315	CLA	C4B-C3B-CAB-CBB
25	b	607	CLA	C4B-C3B-CAB-CBB
25	s	405	CLA	C4B-C3B-CAB-CBB
25	s	417	CLA	C4B-C3B-CAB-CBB
25	r	305	CLA	C4B-C3B-CAB-CBB
25	7	315	CLA	C4B-C3B-CAB-CBB
25	7	317	CLA	C4B-C3B-CAB-CBB
25	B	615	CLA	C15-C16-C17-C18
25	b	606	CLA	C13-C15-C16-C17
30	1	318	LHG	O6-C4-C5-C6
30	a	612	LHG	O6-C4-C5-C6
25	2	315	CLA	O1D-CGD-O2D-CED
30	d	407	LHG	C12-C13-C14-C15
30	2	319	LHG	C23-C24-C25-C26
30	A	601	LHG	C7-C8-C9-C10
30	D	407	LHG	C23-C24-C25-C26
25	g	308	CLA	CBD-CGD-O2D-CED
25	c	609	CLA	CBD-CGD-O2D-CED
24	Y	312	CHL	C13-C15-C16-C17
25	b	603	CLA	C10-C11-C12-C13
24	1	304	CHL	O1D-CGD-O2D-CED
24	p	310	CHL	O1D-CGD-O2D-CED
25	Y	314	CLA	C4-C3-C5-C6
39	D	406	PL9	C45-C44-C46-C47
24	y	313	CHL	C2-C3-C5-C6
30	n	318	LHG	C28-C29-C30-C31
24	9	309	CHL	O1D-CGD-O2D-CED
25	C	602	CLA	C13-C15-C16-C17
25	C	603	CLA	C8-C10-C11-C12
24	r	307	CHL	O1A-CGA-O2A-C1
37	c	619	DGD	C5B-C6B-C7B-C8B
24	G	310	CHL	O1A-CGA-O2A-C1
30	A	612	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	S	608	CHL	C2A-CAA-CBA-CGA
25	B	614	CLA	CBA-CGA-O2A-C1
25	C	606	CLA	CBA-CGA-O2A-C1
30	n	318	LHG	O8-C23-C24-C25
32	A	609	SQD	O47-C7-C8-C9
25	9	316	CLA	C6-C7-C8-C10
30	1	318	LHG	C5-C4-O6-P
30	C	617	LHG	C2-C3-O3-P
30	a	601	LHG	C5-C4-O6-P
30	c	617	LHG	C2-C3-O3-P
24	9	317	CHL	CBD-CGD-O2D-CED
25	9	316	CLA	O1A-CGA-O2A-C1
24	9	311	CHL	C3A-C2A-CAA-CBA
24	Y	304	CHL	C3A-C2A-CAA-CBA
24	u	312	CHL	C3A-C2A-CAA-CBA
24	y	305	CHL	C3A-C2A-CAA-CBA
24	p	305	CHL	C3A-C2A-CAA-CBA
24	s	402	CHL	C3A-C2A-CAA-CBA
24	7	305	CHL	C3A-C2A-CAA-CBA
25	R	612	CLA	C3A-C2A-CAA-CBA
25	8	306	CLA	C3A-C2A-CAA-CBA
25	q	306	CLA	C3A-C2A-CAA-CBA
25	r	313	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C10-C11-C12-C13
29	Y	301	0UR	C46-C47-C48-C49
29	y	301	0UR	C46-C47-C48-C49
33	d	411	LMG	C33-C34-C35-C36
31	D	410	8CT	C16-C17-C18-C19
31	c	613	8CT	C18-C19-C20-C21
30	n	318	LHG	C10-C11-C12-C13
33	W	201	LMG	C30-C31-C32-C33
24	R	601	CHL	O1D-CGD-O2D-CED
25	B	604	CLA	C10-C11-C12-C13
25	B	612	CLA	C10-C11-C12-C13
32	B	618	SQD	C29-C30-C31-C32
32	a	609	SQD	C14-C15-C16-C17
37	C	620	DGD	C5A-C6A-C7A-C8A
25	C	603	CLA	C16-C17-C18-C19
24	3	309	CHL	CBA-CGA-O2A-C1
24	6	309	CHL	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
30	Y	318	LHG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	1	318	LHG	C4-C5-C6-O8
32	D	409	SQD	O6-C44-C45-C46
32	d	409	SQD	O6-C44-C45-C46
33	D	411	LMG	O1-C7-C8-C9
33	w	201	LMG	C7-C8-C9-O8
30	4	318	LHG	C23-C24-C25-C26
32	b	618	SQD	C7-C8-C9-C10
25	c	608	CLA	O1A-CGA-O2A-C1
32	a	609	SQD	C26-C27-C28-C29
25	7	315	CLA	C3-C5-C6-C7
25	B	609	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	b	608	CLA	C6-C7-C8-C9
30	9	318	LHG	C28-C29-C30-C31
30	p	319	LHG	C11-C10-C9-C8
33	d	411	LMG	C13-C14-C15-C16
30	N	318	LHG	C28-C29-C30-C31
25	b	612	CLA	C10-C11-C12-C13
24	1	305	CHL	C3C-C2C-CMC-OMC
24	1	312	CHL	C3C-C2C-CMC-OMC
24	1	317	CHL	C3C-C2C-CMC-OMC
24	2	313	CHL	C3C-C2C-CMC-OMC
24	3	304	CHL	C3C-C2C-CMC-OMC
24	3	311	CHL	C3C-C2C-CMC-OMC
24	3	312	CHL	C3C-C2C-CMC-OMC
24	3	317	CHL	C3C-C2C-CMC-OMC
24	G	310	CHL	C3C-C2C-CMC-OMC
24	9	309	CHL	C3C-C2C-CMC-OMC
24	N	311	CHL	C3C-C2C-CMC-OMC
24	N	317	CHL	C3C-C2C-CMC-OMC
24	8	307	CHL	C3C-C2C-CMC-OMC
24	8	308	CHL	C3C-C2C-CMC-OMC
24	4	305	CHL	C3C-C2C-CMC-OMC
24	4	309	CHL	C3C-C2C-CMC-OMC
24	4	317	CHL	C3C-C2C-CMC-OMC
24	g	310	CHL	C3C-C2C-CMC-OMC
24	u	305	CHL	C3C-C2C-CMC-OMC
24	n	309	CHL	C3C-C2C-CMC-OMC
24	n	311	CHL	C3C-C2C-CMC-OMC
24	n	317	CHL	C3C-C2C-CMC-OMC
24	p	306	CHL	C3C-C2C-CMC-OMC
24	q	307	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	q	308	CHL	C3C-C2C-CMC-OMC
24	s	408	CHL	C3C-C2C-CMC-OMC
24	r	308	CHL	C3C-C2C-CMC-OMC
24	7	306	CHL	C3C-C2C-CMC-OMC
30	9	318	LHG	C4-O6-P-O3
30	C	617	LHG	C3-O3-P-O6
30	D	408	LHG	C4-O6-P-O3
30	c	617	LHG	C3-O3-P-O6
32	B	618	SQD	C7-C8-C9-C10
32	D	409	SQD	C7-C8-C9-C10
24	N	310	CHL	O1A-CGA-O2A-C1
24	8	304	CHL	O1A-CGA-O2A-C1
25	B	613	CLA	O1A-CGA-O2A-C1
25	C	608	CLA	O1A-CGA-O2A-C1
25	p	317	CLA	O1A-CGA-O2A-C1
25	b	604	CLA	C3-C5-C6-C7
25	p	307	CLA	C2A-CAA-CBA-CGA
25	c	601	CLA	C2A-CAA-CBA-CGA
30	C	617	LHG	O1-C1-C2-O2
25	b	605	CLA	C15-C16-C17-C18
25	c	611	CLA	C10-C11-C12-C13
30	c	617	LHG	C11-C10-C9-C8
33	d	411	LMG	C15-C16-C17-C18
30	G	319	LHG	O6-C4-C5-O7
25	8	311	CLA	CBD-CGD-O2D-CED
30	G	319	LHG	C25-C26-C27-C28
30	N	318	LHG	C15-C16-C17-C18
30	7	319	LHG	C11-C10-C9-C8
33	i	101	LMG	C40-C41-C42-C43
24	G	310	CHL	O1D-CGD-O2D-CED
24	R	606	CHL	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
30	d	407	LHG	C23-C24-C25-C26
25	c	602	CLA	C16-C17-C18-C20
25	c	603	CLA	C16-C17-C18-C19
30	g	319	LHG	C25-C26-C27-C28
30	N	318	LHG	O8-C23-C24-C25
24	G	309	CHL	O1D-CGD-O2D-CED
24	p	318	CHL	O1D-CGD-O2D-CED
25	S	616	CLA	C2B-C3B-CAB-CBB
25	Y	306	CLA	C2B-C3B-CAB-CBB
25	4	314	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	6	315	CLA	C2B-C3B-CAB-CBB
25	u	315	CLA	C2B-C3B-CAB-CBB
25	s	405	CLA	C2B-C3B-CAB-CBB
25	s	417	CLA	C2B-C3B-CAB-CBB
25	r	305	CLA	C2B-C3B-CAB-CBB
25	7	317	CLA	C2B-C3B-CAB-CBB
24	q	304	CHL	O1A-CGA-O2A-C1
25	s	413	CLA	O1A-CGA-O2A-C1
24	p	306	CHL	C15-C16-C17-C18
24	7	306	CHL	C15-C16-C17-C18
30	C	617	LHG	O7-C5-C6-O8
30	c	617	LHG	O7-C5-C6-O8
30	d	408	LHG	O7-C5-C6-O8
32	D	409	SQD	O6-C44-C45-O47
33	B	619	LMG	O7-C8-C9-O8
33	D	411	LMG	O1-C7-C8-O7
33	W	201	LMG	O1-C7-C8-O7
33	m	101	LMG	O7-C8-C9-O8
33	w	201	LMG	O7-C8-C9-O8
37	C	620	DGD	O1G-C1G-C2G-O2G
25	B	605	CLA	C15-C16-C17-C18
30	A	601	LHG	C10-C11-C12-C13
37	c	619	DGD	C2B-C3B-C4B-C5B
26	9	303	0IE	C13-C14-C15-C16
30	a	601	LHG	C10-C11-C12-C13
37	c	618	DGD	C3A-C4A-C5A-C6A
32	B	618	SQD	O49-C7-O47-C45
24	S	602	CHL	C2-C1-O2A-CGA
24	G	313	CHL	C2-C1-O2A-CGA
24	N	312	CHL	C2-C1-O2A-CGA
24	Y	305	CHL	C2-C1-O2A-CGA
24	8	303	CHL	C2-C1-O2A-CGA
24	g	311	CHL	C2-C1-O2A-CGA
24	g	313	CHL	C2-C1-O2A-CGA
24	n	312	CHL	C2-C1-O2A-CGA
24	p	305	CHL	C2-C1-O2A-CGA
24	7	305	CHL	C2-C1-O2A-CGA
25	G	308	CLA	C2-C1-O2A-CGA
25	C	603	CLA	C2-C1-O2A-CGA
25	c	603	CLA	C2-C1-O2A-CGA
25	c	607	CLA	C2-C3-C5-C6
30	N	318	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	5	319	LHG	C15-C16-C17-C18
24	n	310	CHL	O1A-CGA-O2A-C1
25	7	317	CLA	O1A-CGA-O2A-C1
25	c	601	CLA	C8-C10-C11-C12
24	g	305	CHL	C11-C10-C8-C9
24	g	313	CHL	C11-C12-C13-C14
24	u	305	CHL	C11-C12-C13-C14
24	y	306	CHL	C14-C13-C15-C16
25	2	315	CLA	C6-C7-C8-C9
25	C	602	CLA	C6-C7-C8-C9
25	y	315	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	G	308	CLA	O1D-CGD-O2D-CED
30	A	601	LHG	C12-C13-C14-C15
25	C	609	CLA	CBD-CGD-O2D-CED
30	C	617	LHG	C11-C10-C9-C8
32	b	618	SQD	C29-C30-C31-C32
33	C	618	LMG	C30-C31-C32-C33
25	5	315	CLA	O1D-CGD-O2D-CED
30	4	318	LHG	C12-C13-C14-C15
32	d	409	SQD	C12-C13-C14-C15
24	1	305	CHL	C2A-CAA-CBA-CGA
25	9	316	CLA	C2A-CAA-CBA-CGA
25	c	605	CLA	C2A-CAA-CBA-CGA
24	r	302	CHL	O1D-CGD-O2D-CED
25	B	608	CLA	C6-C7-C8-C9
25	C	602	CLA	C16-C17-C18-C20
24	1	308	CHL	CBD-CGD-O2D-CED
24	u	305	CHL	C3-C5-C6-C7
25	Y	316	CLA	C11-C10-C8-C7
24	Y	310	CHL	CAA-CBA-CGA-O2A
24	y	310	CHL	CBA-CGA-O2A-C1
30	a	612	LHG	C26-C27-C28-C29
37	C	619	DGD	C3A-C4A-C5A-C6A
24	Y	308	CHL	C1A-C2A-CAA-CBA
24	y	309	CHL	C1A-C2A-CAA-CBA
29	N	301	0UR	C5-C6-C7-C8
29	u	301	0UR	C5-C6-C7-C8
30	D	408	LHG	C27-C28-C29-C30
33	W	201	LMG	O9-C10-O7-C8
30	a	601	LHG	C12-C13-C14-C15
25	9	307	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	G	319	LHG	O6-C4-C5-C6
30	A	612	LHG	O6-C4-C5-C6
30	4	318	LHG	O6-C4-C5-C6
30	p	319	LHG	O6-C4-C5-C6
30	7	319	LHG	O6-C4-C5-C6
24	G	305	CHL	C11-C10-C8-C7
24	G	306	CHL	C12-C13-C15-C16
24	G	313	CHL	C12-C13-C15-C16
24	Y	305	CHL	C11-C10-C8-C7
24	Y	312	CHL	C12-C13-C15-C16
24	g	305	CHL	C11-C10-C8-C7
24	g	306	CHL	C12-C13-C15-C16
24	y	305	CHL	C11-C12-C13-C15
24	y	306	CHL	C12-C13-C15-C16
24	y	313	CHL	C12-C13-C15-C16
24	p	306	CHL	C12-C13-C15-C16
24	7	306	CHL	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C6-C7-C8-C10
25	B	609	CLA	C6-C7-C8-C10
25	B	609	CLA	C11-C10-C8-C7
25	B	609	CLA	C12-C13-C15-C16
25	B	612	CLA	C11-C12-C13-C15
25	B	614	CLA	C6-C7-C8-C10
25	C	602	CLA	C12-C13-C15-C16
25	C	607	CLA	C2-C3-C5-C6
25	C	611	CLA	C11-C10-C8-C7
25	5	315	CLA	C6-C7-C8-C10
25	y	315	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	603	CLA	C12-C13-C15-C16
25	b	604	CLA	C6-C7-C8-C10
25	b	606	CLA	C11-C10-C8-C7
25	b	609	CLA	C11-C10-C8-C7
25	b	612	CLA	C11-C12-C13-C15
25	b	614	CLA	C6-C7-C8-C10
25	c	601	CLA	C12-C13-C15-C16
25	c	602	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C10-C8-C7
29	1	301	0UR	C46-C47-C48-C49
29	2	301	0UR	C46-C47-C48-C49
29	3	301	0UR	C46-C47-C48-C49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	G	301	0UR	C46-C47-C48-C49
29	N	301	0UR	C46-C47-C48-C49
29	4	301	0UR	C46-C47-C48-C49
29	5	301	0UR	C46-C47-C48-C49
29	g	301	0UR	C46-C47-C48-C49
30	G	319	LHG	C11-C10-C9-C8
30	5	319	LHG	C10-C11-C12-C13
29	p	301	0UR	C3-C4-C5-C6
31	B	617	8CT	C12-C13-C14-C15
31	C	613	8CT	C18-C19-C20-C21
31	b	617	8CT	C12-C13-C14-C15
31	d	410	8CT	C16-C17-C18-C19
25	y	317	CLA	C11-C10-C8-C7
32	b	618	SQD	O49-C7-O47-C45
25	8	305	CLA	CBA-CGA-O2A-C1
25	S	612	CLA	O1A-CGA-O2A-C1
24	R	602	CHL	C2A-CAA-CBA-CGA
24	s	409	CHL	C2A-CAA-CBA-CGA
24	r	303	CHL	C2A-CAA-CBA-CGA
25	A	603	CLA	C2A-CAA-CBA-CGA
25	u	308	CLA	C2A-CAA-CBA-CGA
25	a	603	CLA	C2A-CAA-CBA-CGA
26	1	302	0IE	O1-C2-C3-C4
26	2	302	0IE	O1-C2-C3-C4
26	3	302	0IE	O1-C2-C3-C4
26	G	302	0IE	O1-C2-C3-C4
26	9	302	0IE	O1-C2-C3-C4
26	N	302	0IE	O1-C2-C3-C4
26	Y	302	0IE	O1-C2-C3-C4
26	8	302	0IE	O1-C2-C3-C4
26	4	302	0IE	O1-C2-C3-C4
26	5	302	0IE	O1-C2-C3-C4
26	6	302	0IE	O1-C2-C3-C4
26	g	302	0IE	O1-C2-C3-C4
26	u	302	0IE	O1-C2-C3-C4
26	n	302	0IE	O1-C2-C3-C4
26	y	302	0IE	O1-C2-C3-C4
26	p	302	0IE	O1-C2-C3-C4
26	q	302	0IE	O1-C2-C3-C4
26	7	302	0IE	O1-C2-C3-C4
29	1	301	0UR	O42-C2-C3-C4
29	2	301	0UR	O42-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	G	301	0UR	O42-C2-C3-C4
29	9	301	0UR	O42-C2-C3-C4
29	Y	301	0UR	O42-C2-C3-C4
29	8	301	0UR	O42-C2-C3-C4
29	4	301	0UR	O42-C2-C3-C4
29	5	301	0UR	O42-C2-C3-C4
29	g	301	0UR	O42-C2-C3-C4
29	u	301	0UR	O42-C2-C3-C4
29	y	301	0UR	O42-C2-C3-C4
29	q	301	0UR	O42-C2-C3-C4
32	A	609	SQD	C26-C27-C28-C29
25	p	315	CLA	C3-C5-C6-C7
24	N	312	CHL	CBA-CGA-O2A-C1
25	2	317	CLA	CBA-CGA-O2A-C1
25	c	606	CLA	CBA-CGA-O2A-C1
33	C	618	LMG	C13-C14-C15-C16
24	7	310	CHL	O1D-CGD-O2D-CED
25	g	315	CLA	C5-C6-C7-C8
25	b	609	CLA	C10-C11-C12-C13
25	d	404	CLA	C10-C11-C12-C13
29	n	301	0UR	C46-C47-C48-C49
24	u	310	CHL	CBD-CGD-O2D-CED
25	c	612	CLA	CBD-CGD-O2D-CED
24	2	309	CHL	CAD-CBD-CGD-O2D
24	5	309	CHL	CAD-CBD-CGD-O2D
24	q	316	CHL	CAD-CBD-CGD-O2D
24	r	308	CHL	CAD-CBD-CGD-O2D
25	1	316	CLA	CAD-CBD-CGD-O2D
25	S	604	CLA	CAD-CBD-CGD-O2D
25	S	609	CLA	CAD-CBD-CGD-O2D
25	G	314	CLA	CAD-CBD-CGD-O2D
25	9	314	CLA	CAD-CBD-CGD-O2D
25	N	307	CLA	CAD-CBD-CGD-O2D
25	Y	313	CLA	CAD-CBD-CGD-O2D
25	8	311	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	C	604	CLA	CAD-CBD-CGD-O2D
25	C	609	CLA	CAD-CBD-CGD-O2D
25	g	314	CLA	CAD-CBD-CGD-O2D
25	u	315	CLA	CAD-CBD-CGD-O2D
25	y	314	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	613	CLA	CAD-CBD-CGD-O2D
25	c	604	CLA	CAD-CBD-CGD-O2D
25	c	609	CLA	CAD-CBD-CGD-O2D
25	d	404	CLA	CAD-CBD-CGD-O2D
25	s	405	CLA	CAD-CBD-CGD-O2D
25	s	410	CLA	CAD-CBD-CGD-O2D
33	d	411	LMG	C34-C35-C36-C37
30	D	407	LHG	C28-C29-C30-C31
33	w	201	LMG	C14-C15-C16-C17
25	q	305	CLA	CBA-CGA-O2A-C1
25	B	605	CLA	C4-C3-C5-C6
25	b	609	CLA	C4-C3-C5-C6
24	8	310	CHL	C6-C7-C8-C9
24	q	311	CHL	C6-C7-C8-C9
33	d	411	LMG	C19-C20-C21-C22
33	m	101	LMG	C7-C8-C9-O8
37	C	619	DGD	O1G-C1G-C2G-C3G
37	C	620	DGD	C1G-C2G-C3G-O3G
25	q	305	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	O1A-CGA-O2A-C1
30	9	318	LHG	O6-C4-C5-O7
30	a	612	LHG	O6-C4-C5-O7
25	n	314	CLA	C5-C6-C7-C8
25	2	317	CLA	O2A-C1-C2-C3
25	5	317	CLA	O2A-C1-C2-C3
30	2	319	LHG	C10-C11-C12-C13
25	C	605	CLA	C2A-CAA-CBA-CGA
32	D	409	SQD	C9-C10-C11-C12
33	D	411	LMG	C19-C20-C21-C22
37	c	619	DGD	C1B-C2B-C3B-C4B
29	6	301	0UR	C46-C47-C48-C49
24	R	602	CHL	CHA-CBD-CGD-O1D
24	R	602	CHL	CHA-CBD-CGD-O2D
24	N	305	CHL	CHA-CBD-CGD-O1D
24	N	308	CHL	CHA-CBD-CGD-O1D
24	N	308	CHL	CHA-CBD-CGD-O2D
24	Y	317	CHL	CHA-CBD-CGD-O1D
24	Y	317	CHL	CHA-CBD-CGD-O2D
24	g	313	CHL	CHA-CBD-CGD-O2D
24	n	305	CHL	CHA-CBD-CGD-O1D
24	n	305	CHL	CHA-CBD-CGD-O2D
24	y	318	CHL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	y	318	CHL	CHA-CBD-CGD-O2D
24	p	318	CHL	CHA-CBD-CGD-O1D
24	p	318	CHL	CHA-CBD-CGD-O2D
24	r	303	CHL	CHA-CBD-CGD-O1D
24	r	303	CHL	CHA-CBD-CGD-O2D
24	7	318	CHL	CHA-CBD-CGD-O1D
24	7	318	CHL	CHA-CBD-CGD-O2D
25	R	603	CLA	CHA-CBD-CGD-O1D
25	R	603	CLA	CHA-CBD-CGD-O2D
25	R	613	CLA	CHA-CBD-CGD-O1D
25	R	613	CLA	CHA-CBD-CGD-O2D
25	1	314	CLA	CHA-CBD-CGD-O1D
25	1	314	CLA	CHA-CBD-CGD-O2D
25	1	315	CLA	CHA-CBD-CGD-O1D
25	1	315	CLA	CHA-CBD-CGD-O2D
25	2	316	CLA	CHA-CBD-CGD-O1D
25	2	316	CLA	CHA-CBD-CGD-O2D
25	S	611	CLA	CHA-CBD-CGD-O1D
25	S	611	CLA	CHA-CBD-CGD-O2D
25	9	315	CLA	CHA-CBD-CGD-O1D
25	N	306	CLA	CHA-CBD-CGD-O1D
25	N	306	CLA	CHA-CBD-CGD-O2D
25	8	305	CLA	CHA-CBD-CGD-O1D
25	8	305	CLA	CHA-CBD-CGD-O2D
25	8	313	CLA	CHA-CBD-CGD-O1D
25	8	313	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	616	CLA	CHA-CBD-CGD-O1D
25	A	610	CLA	CHA-CBD-CGD-O1D
25	A	610	CLA	CHA-CBD-CGD-O2D
25	C	607	CLA	CHA-CBD-CGD-O1D
25	C	608	CLA	CHA-CBD-CGD-O1D
25	C	608	CLA	CHA-CBD-CGD-O2D
25	4	314	CLA	CHA-CBD-CGD-O1D
25	4	314	CLA	CHA-CBD-CGD-O2D
25	4	315	CLA	CHA-CBD-CGD-O1D
25	4	315	CLA	CHA-CBD-CGD-O2D
25	5	316	CLA	CHA-CBD-CGD-O1D
25	5	316	CLA	CHA-CBD-CGD-O2D
25	g	316	CLA	CHA-CBD-CGD-O1D
25	u	308	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	u	316	CLA	CHA-CBD-CGD-O1D
25	u	316	CLA	CHA-CBD-CGD-O2D
25	u	317	CLA	CHA-CBD-CGD-O1D
25	u	317	CLA	CHA-CBD-CGD-O2D
25	n	306	CLA	CHA-CBD-CGD-O1D
25	n	306	CLA	CHA-CBD-CGD-O2D
25	p	307	CLA	CHA-CBD-CGD-O1D
25	p	307	CLA	CHA-CBD-CGD-O2D
25	p	308	CLA	CHA-CBD-CGD-O1D
25	p	316	CLA	CHA-CBD-CGD-O1D
25	p	316	CLA	CHA-CBD-CGD-O2D
25	p	317	CLA	CHA-CBD-CGD-O1D
25	q	305	CLA	CHA-CBD-CGD-O1D
25	q	305	CLA	CHA-CBD-CGD-O2D
25	q	314	CLA	CHA-CBD-CGD-O1D
25	q	314	CLA	CHA-CBD-CGD-O2D
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	602	CLA	CHA-CBD-CGD-O2D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	a	610	CLA	CHA-CBD-CGD-O1D
25	a	610	CLA	CHA-CBD-CGD-O2D
25	c	604	CLA	CHA-CBD-CGD-O1D
25	c	608	CLA	CHA-CBD-CGD-O1D
25	c	608	CLA	CHA-CBD-CGD-O2D
25	s	412	CLA	CHA-CBD-CGD-O1D
25	s	412	CLA	CHA-CBD-CGD-O2D
25	r	304	CLA	CHA-CBD-CGD-O1D
25	r	304	CLA	CHA-CBD-CGD-O2D
25	r	312	CLA	CHA-CBD-CGD-O1D
25	r	314	CLA	CHA-CBD-CGD-O1D
25	r	314	CLA	CHA-CBD-CGD-O2D
25	7	307	CLA	CHA-CBD-CGD-O1D
25	7	307	CLA	CHA-CBD-CGD-O2D
25	7	308	CLA	CHA-CBD-CGD-O1D
25	7	315	CLA	CHA-CBD-CGD-O1D
25	7	316	CLA	CHA-CBD-CGD-O1D
25	7	316	CLA	CHA-CBD-CGD-O2D
25	7	317	CLA	CHA-CBD-CGD-O1D
25	7	317	CLA	CHA-CBD-CGD-O2D
32	D	409	SQD	C27-C28-C29-C30
24	9	304	CHL	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	6	309	CHL	O1A-CGA-O2A-C1
25	C	606	CLA	O1A-CGA-O2A-C1
32	B	618	SQD	O6-C44-C45-O47
32	d	409	SQD	O6-C44-C45-O47
37	C	619	DGD	O1G-C1G-C2G-O2G
37	C	620	DGD	O2G-C2G-C3G-O3G
25	5	317	CLA	CBA-CGA-O2A-C1
24	3	309	CHL	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
37	c	618	DGD	C2B-C3B-C4B-C5B
30	c	617	LHG	O1-C1-C2-O2
24	2	313	CHL	O1D-CGD-O2D-CED
24	5	313	CHL	O1D-CGD-O2D-CED
25	C	612	CLA	O1D-CGD-O2D-CED
33	B	619	LMG	C16-C17-C18-C19
30	D	407	LHG	C12-C13-C14-C15
24	2	311	CHL	CAA-CBA-CGA-O2A
24	Y	312	CHL	C14-C13-C15-C16
24	y	313	CHL	C14-C13-C15-C16
24	p	306	CHL	C14-C13-C15-C16
25	c	602	CLA	C6-C7-C8-C9
37	C	620	DGD	C4D-C5D-C6D-O5D
24	N	312	CHL	O1A-CGA-O2A-C1
25	B	607	CLA	C10-C11-C12-C13
25	b	615	CLA	C5-C6-C7-C8
26	7	303	0IE	O29-C20-C3-C4
24	3	310	CHL	C2A-CAA-CBA-CGA
25	G	317	CLA	C2A-CAA-CBA-CGA
25	c	608	CLA	C14-C13-C15-C16
25	8	305	CLA	O1A-CGA-O2A-C1
25	c	606	CLA	O1A-CGA-O2A-C1
31	D	410	8CT	C10-C11-C12-C40
24	q	311	CHL	C2C-C3C-CAC-CBC
30	a	612	LHG	C14-C15-C16-C17
37	C	619	DGD	C2B-C3B-C4B-C5B
26	9	303	0IE	C11-C12-C13-C14
29	1	301	0UR	C15-C16-C17-C18
29	y	301	0UR	C5-C6-C7-C8
31	X	601	8CT	C25-C26-C28-C29
24	u	310	CHL	O1D-CGD-O2D-CED
24	7	318	CHL	O1D-CGD-O2D-CED
24	u	310	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	p	305	CHL	C1A-C2A-CAA-CBA
24	s	402	CHL	C1A-C2A-CAA-CBA
24	7	305	CHL	C1A-C2A-CAA-CBA
25	9	313	CLA	C1A-C2A-CAA-CBA
25	8	306	CLA	C1A-C2A-CAA-CBA
25	A	605	CLA	C1A-C2A-CAA-CBA
25	C	601	CLA	C1A-C2A-CAA-CBA
25	u	314	CLA	C1A-C2A-CAA-CBA
25	a	605	CLA	C1A-C2A-CAA-CBA
25	c	601	CLA	C1A-C2A-CAA-CBA
24	N	312	CHL	C6-C7-C8-C9
24	n	312	CHL	C6-C7-C8-C9
25	D	405	CLA	C16-C17-C18-C20
25	d	405	CLA	C16-C17-C18-C20
33	D	401	LMG	C12-C13-C14-C15
29	7	301	0UR	C46-C47-C48-C49
24	s	403	CHL	CBA-CGA-O2A-C1
25	G	308	CLA	CBA-CGA-O2A-C1
32	d	409	SQD	C9-C10-C11-C12
29	3	301	0UR	C3-C4-C5-C6
35	d	403	PHO	O1D-CGD-O2D-CED
30	y	319	LHG	C4-O6-P-O3
25	8	305	CLA	CBD-CGD-O2D-CED
30	A	612	LHG	C14-C15-C16-C17
25	B	604	CLA	C3-C5-C6-C7
30	A	612	LHG	C2-C3-O3-P
30	a	612	LHG	C2-C3-O3-P
25	c	610	CLA	C2-C3-C5-C6
24	8	310	CHL	C2C-C3C-CAC-CBC
24	9	305	CHL	C4B-C3B-CAB-CBB
24	u	306	CHL	C4B-C3B-CAB-CBB
24	n	305	CHL	C4B-C3B-CAB-CBB
24	p	305	CHL	C4B-C3B-CAB-CBB
24	p	306	CHL	C4B-C3B-CAB-CBB
24	7	305	CHL	C4B-C3B-CAB-CBB
24	7	306	CHL	C4B-C3B-CAB-CBB
25	R	612	CLA	C4B-C3B-CAB-CBB
25	1	315	CLA	C4B-C3B-CAB-CBB
25	2	315	CLA	C4B-C3B-CAB-CBB
25	3	315	CLA	C4B-C3B-CAB-CBB
25	9	314	CLA	C4B-C3B-CAB-CBB
25	4	315	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	5	315	CLA	C4B-C3B-CAB-CBB
25	6	315	CLA	C4B-C3B-CAB-CBB
25	6	316	CLA	C4B-C3B-CAB-CBB
25	p	317	CLA	C4B-C3B-CAB-CBB
25	r	313	CLA	C4B-C3B-CAB-CBB
30	G	319	LHG	C3-O3-P-O4
30	9	318	LHG	C3-O3-P-O4
30	A	601	LHG	C3-O3-P-O4
30	A	601	LHG	C3-O3-P-O5
30	C	617	LHG	C4-O6-P-O4
30	D	407	LHG	C4-O6-P-O4
30	D	408	LHG	C3-O3-P-O4
30	g	319	LHG	C3-O3-P-O4
30	g	319	LHG	C4-O6-P-O4
30	p	319	LHG	C3-O3-P-O4
30	a	601	LHG	C3-O3-P-O4
30	a	601	LHG	C3-O3-P-O5
30	c	617	LHG	C4-O6-P-O4
30	d	407	LHG	C4-O6-P-O4
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C4-O6-P-O4
30	7	319	LHG	C3-O3-P-O4
25	c	601	CLA	C16-C17-C18-C20
30	A	612	LHG	C27-C28-C29-C30
24	n	312	CHL	CBA-CGA-O2A-C1
24	9	311	CHL	O1A-CGA-O2A-C1
24	1	308	CHL	O1D-CGD-O2D-CED
24	9	317	CHL	O1D-CGD-O2D-CED
25	B	602	CLA	CAA-CBA-CGA-O2A
25	G	315	CLA	C5-C6-C7-C8
25	b	607	CLA	C10-C11-C12-C13
25	g	317	CLA	C2A-CAA-CBA-CGA
25	g	317	CLA	C3-C5-C6-C7
25	8	311	CLA	O1D-CGD-O2D-CED
30	n	318	LHG	C26-C27-C28-C29
33	d	411	LMG	C20-C21-C22-C23
24	Y	317	CHL	CAD-CBD-CGD-O1D
24	y	318	CHL	CAD-CBD-CGD-O1D
24	p	318	CHL	CAD-CBD-CGD-O1D
24	7	318	CHL	CAD-CBD-CGD-O1D
25	C	602	CLA	CAD-CBD-CGD-O1D
25	C	605	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	405	CLA	CAD-CBD-CGD-O1D
25	p	308	CLA	CAD-CBD-CGD-O1D
25	c	602	CLA	CAD-CBD-CGD-O1D
25	c	605	CLA	CAD-CBD-CGD-O1D
25	d	405	CLA	CAD-CBD-CGD-O1D
25	7	308	CLA	CAD-CBD-CGD-O1D
24	5	311	CHL	CAA-CBA-CGA-O2A
37	C	620	DGD	O6D-C5D-C6D-O5D
30	1	318	LHG	C11-C10-C9-C8
30	N	318	LHG	C26-C27-C28-C29
24	S	602	CHL	CBA-CGA-O2A-C1
24	N	308	CHL	O1D-CGD-O2D-CED
25	g	308	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	C4-C3-C5-C6
25	c	609	CLA	O1D-CGD-O2D-CED
24	S	601	CHL	C3A-C2A-CAA-CBA
24	7	306	CHL	C12-C13-C15-C16
25	2	315	CLA	C11-C12-C13-C15
25	Y	314	CLA	C6-C7-C8-C10
25	B	604	CLA	C11-C12-C13-C15
25	A	604	CLA	C3A-C2A-CAA-CBA
25	C	608	CLA	C6-C7-C8-C10
25	5	315	CLA	C11-C12-C13-C15
25	a	604	CLA	C3A-C2A-CAA-CBA
25	c	608	CLA	C6-C7-C8-C10
25	d	404	CLA	C11-C12-C13-C15
26	3	302	0IE	O29-C20-C3-C2
26	9	302	0IE	O29-C20-C3-C2
26	6	302	0IE	O29-C20-C3-C2
26	g	302	0IE	O1-C2-C3-C20
26	u	302	0IE	O29-C20-C3-C2
26	u	303	0IE	O29-C20-C3-C2
26	p	302	0IE	O29-C20-C3-C2
26	p	303	0IE	O29-C20-C3-C2
26	7	302	0IE	O29-C20-C3-C2
26	7	303	0IE	O29-C20-C3-C2
29	8	301	0UR	O42-C2-C3-C43
29	q	301	0UR	O42-C2-C3-C43
30	1	318	LHG	O6-C4-C5-O7
30	4	318	LHG	O6-C4-C5-O7
30	g	319	LHG	O6-C4-C5-O7
31	T	101	8CT	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	t	101	8CT	C28-C29-C30-C31
31	c	613	8CT	C28-C29-C30-C31
30	D	407	LHG	C31-C32-C33-C34
32	D	409	SQD	C12-C13-C14-C15
29	p	301	0UR	C46-C47-C48-C49
25	q	305	CLA	O1A-CGA-O2A-C1
35	D	403	PHO	CBD-CGD-O2D-CED
24	g	311	CHL	CAA-CBA-CGA-O2A
25	2	317	CLA	O1A-CGA-O2A-C1
30	4	318	LHG	C27-C28-C29-C30
24	u	312	CHL	O1A-CGA-O2A-C1
25	g	308	CLA	C2A-CAA-CBA-CGA
25	u	317	CLA	C2A-CAA-CBA-CGA
25	C	601	CLA	C16-C17-C18-C20
32	A	609	SQD	C28-C29-C30-C31
33	m	101	LMG	C28-C29-C30-C31
25	b	602	CLA	CAA-CBA-CGA-O2A
32	a	609	SQD	O47-C7-C8-C9
24	R	601	CHL	C1C-C2C-CMC-OMC
24	R	607	CHL	C1C-C2C-CMC-OMC
24	1	305	CHL	C1C-C2C-CMC-OMC
24	1	312	CHL	C1C-C2C-CMC-OMC
24	1	317	CHL	C1C-C2C-CMC-OMC
24	2	305	CHL	C1C-C2C-CMC-OMC
24	2	306	CHL	C1C-C2C-CMC-OMC
24	2	312	CHL	C1C-C2C-CMC-OMC
24	2	313	CHL	C1C-C2C-CMC-OMC
24	3	304	CHL	C1C-C2C-CMC-OMC
24	3	311	CHL	C1C-C2C-CMC-OMC
24	3	312	CHL	C1C-C2C-CMC-OMC
24	3	317	CHL	C1C-C2C-CMC-OMC
24	S	602	CHL	C1C-C2C-CMC-OMC
24	S	608	CHL	C1C-C2C-CMC-OMC
24	S	613	CHL	C1C-C2C-CMC-OMC
24	G	306	CHL	C1C-C2C-CMC-OMC
24	G	310	CHL	C1C-C2C-CMC-OMC
24	G	318	CHL	C1C-C2C-CMC-OMC
24	9	304	CHL	C1C-C2C-CMC-OMC
24	9	309	CHL	C1C-C2C-CMC-OMC
24	N	305	CHL	C1C-C2C-CMC-OMC
24	N	309	CHL	C1C-C2C-CMC-OMC
24	N	311	CHL	C1C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	N	312	CHL	C1C-C2C-CMC-OMC
24	N	317	CHL	C1C-C2C-CMC-OMC
24	Y	308	CHL	C1C-C2C-CMC-OMC
24	Y	310	CHL	C1C-C2C-CMC-OMC
24	Y	317	CHL	C1C-C2C-CMC-OMC
24	8	304	CHL	C1C-C2C-CMC-OMC
24	8	307	CHL	C1C-C2C-CMC-OMC
24	8	308	CHL	C1C-C2C-CMC-OMC
24	8	310	CHL	C1C-C2C-CMC-OMC
24	4	305	CHL	C1C-C2C-CMC-OMC
24	4	309	CHL	C1C-C2C-CMC-OMC
24	4	312	CHL	C1C-C2C-CMC-OMC
24	4	317	CHL	C1C-C2C-CMC-OMC
24	5	305	CHL	C1C-C2C-CMC-OMC
24	5	306	CHL	C1C-C2C-CMC-OMC
24	5	312	CHL	C1C-C2C-CMC-OMC
24	6	304	CHL	C1C-C2C-CMC-OMC
24	g	306	CHL	C1C-C2C-CMC-OMC
24	g	310	CHL	C1C-C2C-CMC-OMC
24	g	318	CHL	C1C-C2C-CMC-OMC
24	u	310	CHL	C1C-C2C-CMC-OMC
24	n	305	CHL	C1C-C2C-CMC-OMC
24	n	309	CHL	C1C-C2C-CMC-OMC
24	n	311	CHL	C1C-C2C-CMC-OMC
24	n	312	CHL	C1C-C2C-CMC-OMC
24	n	317	CHL	C1C-C2C-CMC-OMC
24	y	309	CHL	C1C-C2C-CMC-OMC
24	y	311	CHL	C1C-C2C-CMC-OMC
24	y	312	CHL	C1C-C2C-CMC-OMC
24	y	318	CHL	C1C-C2C-CMC-OMC
24	q	304	CHL	C1C-C2C-CMC-OMC
24	q	307	CHL	C1C-C2C-CMC-OMC
24	q	308	CHL	C1C-C2C-CMC-OMC
24	q	311	CHL	C1C-C2C-CMC-OMC
24	s	403	CHL	C1C-C2C-CMC-OMC
24	s	409	CHL	C1C-C2C-CMC-OMC
24	s	414	CHL	C1C-C2C-CMC-OMC
24	r	302	CHL	C1C-C2C-CMC-OMC
24	r	306	CHL	C1C-C2C-CMC-OMC
24	r	308	CHL	C1C-C2C-CMC-OMC
30	d	408	LHG	C4-C5-C6-O8
33	C	618	LMG	O1-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	W	201	LMG	O1-C7-C8-C9
37	c	618	DGD	O1G-C1G-C2G-C3G
32	b	618	SQD	O6-C44-C45-O47
33	D	411	LMG	O7-C8-C9-O8
33	i	101	LMG	O7-C8-C9-O8
37	c	618	DGD	O1G-C1G-C2G-O2G
30	d	408	LHG	C27-C28-C29-C30
30	a	612	LHG	C27-C28-C29-C30
24	s	403	CHL	O1A-CGA-O2A-C1
25	G	308	CLA	O1A-CGA-O2A-C1
29	8	301	0UR	C46-C47-C48-C49
29	q	301	0UR	C46-C47-C48-C49
30	D	407	LHG	C17-C18-C19-C20
33	D	411	LMG	C8-C7-O1-C1
33	d	411	LMG	C8-C7-O1-C1
37	C	619	DGD	C2G-C3G-O3G-C1D
37	C	619	DGD	C5D-C6D-O5D-C1E
37	c	618	DGD	C2G-C3G-O3G-C1D
37	c	618	DGD	C5D-C6D-O5D-C1E
25	5	314	CLA	C3-C5-C6-C7
24	2	306	CHL	CBA-CGA-O2A-C1
24	5	306	CHL	CBA-CGA-O2A-C1
24	r	308	CHL	CBA-CGA-O2A-C1
33	C	618	LMG	C11-C12-C13-C14
24	q	309	CHL	CAA-CBA-CGA-O2A
24	Y	304	CHL	C11-C12-C13-C14
24	g	313	CHL	C6-C7-C8-C9
24	n	305	CHL	C11-C10-C8-C9
24	7	306	CHL	C14-C13-C15-C16
25	8	312	CLA	C11-C10-C8-C9
25	B	612	CLA	C11-C12-C13-C14
25	C	601	CLA	C11-C12-C13-C14
25	C	602	CLA	C14-C13-C15-C16
25	D	405	CLA	C11-C10-C8-C9
25	y	315	CLA	C11-C10-C8-C9
25	y	315	CLA	C14-C13-C15-C16
25	q	313	CLA	C11-C10-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	612	CLA	C11-C12-C13-C14
25	c	602	CLA	C14-C13-C15-C16
24	n	312	CHL	O1A-CGA-O2A-C1
24	G	313	CHL	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	2	314	CLA	C3-C5-C6-C7
25	B	606	CLA	C3-C5-C6-C7
30	a	601	LHG	C29-C30-C31-C32
33	d	401	LMG	C13-C14-C15-C16
32	A	609	SQD	C16-C17-C18-C19
24	S	602	CHL	O1A-CGA-O2A-C1
25	5	317	CLA	O1A-CGA-O2A-C1
25	q	306	CLA	C2A-CAA-CBA-CGA
25	7	307	CLA	C2A-CAA-CBA-CGA
24	Y	319	CHL	CAA-CBA-CGA-O2A
30	9	318	LHG	O1-C1-C2-O2
25	b	604	CLA	C10-C11-C12-C13
31	S	614	8CT	C13-C14-C15-C16
31	S	615	8CT	C13-C14-C15-C16
31	s	415	8CT	C13-C14-C15-C16
31	s	416	8CT	C13-C14-C15-C16
30	a	601	LHG	C9-C10-C11-C12
29	2	301	0UR	C41-C2-C3-C4
29	G	301	0UR	C41-C2-C3-C4
29	Y	301	0UR	C41-C2-C3-C4
29	5	301	0UR	C41-C2-C3-C4
29	g	301	0UR	C41-C2-C3-C4
29	y	301	0UR	C41-C2-C3-C4
25	u	317	CLA	C6-C7-C8-C10
25	C	609	CLA	O1D-CGD-O2D-CED
31	x	601	8CT	C25-C26-C28-C29
25	C	602	CLA	C8-C10-C11-C12
30	D	407	LHG	C30-C31-C32-C33
24	y	311	CHL	C2B-C3B-CAB-CBB
25	R	604	CLA	C2B-C3B-CAB-CBB
25	1	314	CLA	C2B-C3B-CAB-CBB
25	2	307	CLA	C2B-C3B-CAB-CBB
25	3	315	CLA	C2B-C3B-CAB-CBB
25	9	306	CLA	C2B-C3B-CAB-CBB
25	9	314	CLA	C2B-C3B-CAB-CBB
25	9	315	CLA	C2B-C3B-CAB-CBB
25	N	306	CLA	C2B-C3B-CAB-CBB
25	8	305	CLA	C2B-C3B-CAB-CBB
25	4	315	CLA	C2B-C3B-CAB-CBB
25	5	307	CLA	C2B-C3B-CAB-CBB
25	u	307	CLA	C2B-C3B-CAB-CBB
25	n	306	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	p	315	CLA	C2B-C3B-CAB-CBB
25	p	317	CLA	C2B-C3B-CAB-CBB
25	q	305	CLA	C2B-C3B-CAB-CBB
25	r	312	CLA	C2B-C3B-CAB-CBB
25	r	313	CLA	C2B-C3B-CAB-CBB
25	7	315	CLA	C2B-C3B-CAB-CBB
32	B	618	SQD	C8-C7-O47-C45
30	p	319	LHG	C31-C32-C33-C34
32	B	618	SQD	O47-C7-C8-C9
25	B	615	CLA	C5-C6-C7-C8
25	B	609	CLA	C16-C17-C18-C20
25	c	601	CLA	C16-C17-C18-C19
33	C	618	LMG	C34-C35-C36-C37
24	N	311	CHL	C1-C2-C3-C4
24	8	309	CHL	C1-C2-C3-C4
24	n	311	CHL	C1-C2-C3-C4
24	q	310	CHL	C1-C2-C3-C4
25	2	317	CLA	C1-C2-C3-C4
25	5	317	CLA	C1-C2-C3-C4
33	B	619	LMG	O6-C5-C6-O5
32	b	618	SQD	O47-C7-C8-C9
37	C	619	DGD	C3G-C2G-O2G-C1B
30	g	319	LHG	O6-C4-C5-C6
24	4	305	CHL	C2A-CAA-CBA-CGA
24	u	305	CHL	C2A-CAA-CBA-CGA
25	8	306	CLA	C2A-CAA-CBA-CGA
25	6	316	CLA	C2A-CAA-CBA-CGA
25	n	313	CLA	C2A-CAA-CBA-CGA
25	p	317	CLA	C2A-CAA-CBA-CGA
25	7	317	CLA	C2A-CAA-CBA-CGA
30	7	319	LHG	C9-C10-C11-C12
24	G	311	CHL	C2-C1-O2A-CGA
24	Y	312	CHL	C2-C1-O2A-CGA
24	y	306	CHL	C2-C1-O2A-CGA
24	p	306	CHL	C2-C1-O2A-CGA
24	q	303	CHL	C2-C1-O2A-CGA
33	C	618	LMG	C10-C11-C12-C13
37	C	619	DGD	C1B-C2B-C3B-C4B
37	c	618	DGD	C1B-C2B-C3B-C4B
24	r	308	CHL	O1A-CGA-O2A-C1
32	D	409	SQD	C14-C15-C16-C17
24	S	608	CHL	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	5	311	CHL	O1A-CGA-O2A-C1
30	D	407	LHG	C2-C3-O3-P
37	c	619	DGD	C4D-C5D-C6D-O5D
30	D	408	LHG	C11-C10-C9-C8
35	D	403	PHO	O1D-CGD-O2D-CED
25	y	315	CLA	C4-C3-C5-C6
24	3	310	CHL	CBD-CGD-O2D-CED
24	n	305	CHL	C11-C12-C13-C14
31	C	615	8CT	C04-C03-C10-C11
24	3	310	CHL	O1D-CGD-O2D-CED
24	S	608	CHL	O1D-CGD-O2D-CED
30	7	319	LHG	C31-C32-C33-C34
32	D	409	SQD	O47-C7-C8-C9
32	d	409	SQD	O47-C7-C8-C9
32	b	618	SQD	C8-C7-O47-C45
37	c	618	DGD	C7B-C8B-C9B-CAB
24	y	311	CHL	CAA-CBA-CGA-O2A
33	C	618	LMG	O1-C7-C8-O7
33	d	411	LMG	O1-C7-C8-O7
24	s	409	CHL	C4C-C3C-CAC-CBC
30	D	408	LHG	C31-C32-C33-C34
30	N	318	LHG	C3-O3-P-O6
30	Y	318	LHG	C3-O3-P-O6
30	Y	318	LHG	C4-O6-P-O3
30	A	612	LHG	C4-O6-P-O3
30	n	318	LHG	C3-O3-P-O6
30	y	319	LHG	C3-O3-P-O6
30	a	612	LHG	C4-O6-P-O3
33	B	619	LMG	C10-C11-C12-C13
37	C	619	DGD	C7B-C8B-C9B-CAB
24	2	311	CHL	O1A-CGA-O2A-C1
24	N	309	CHL	O1D-CGD-O2D-CED
24	q	309	CHL	O1D-CGD-O2D-CED
25	s	413	CLA	C4-C3-C5-C6
30	d	407	LHG	C11-C12-C13-C14
30	d	407	LHG	C17-C18-C19-C20
25	S	612	CLA	C2-C3-C5-C6
25	B	606	CLA	C11-C10-C8-C7
25	C	608	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C12-C13-C15
25	n	306	CLA	C6-C7-C8-C9
24	G	313	CHL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	g	313	CHL	C14-C13-C15-C16
25	2	315	CLA	C11-C12-C13-C14
25	B	609	CLA	C6-C7-C8-C9
25	5	315	CLA	C11-C12-C13-C14
25	c	608	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C12-C13-C14
25	d	405	CLA	C11-C10-C8-C9
35	d	403	PHO	C11-C12-C13-C14
29	6	301	0UR	C3-C4-C5-C6
31	d	410	8CT	C12-C13-C14-C15
33	i	101	LMG	C12-C13-C14-C15
25	b	606	CLA	C15-C16-C17-C18
25	G	307	CLA	C2A-CAA-CBA-CGA
25	C	601	CLA	C16-C17-C18-C19
30	d	407	LHG	C2-C3-O3-P
24	r	309	CHL	C2C-C3C-CAC-CBC
32	b	618	SQD	C16-C17-C18-C19
29	u	301	0UR	C46-C47-C48-C49
24	g	310	CHL	O1D-CGD-O2D-CED
29	Y	301	0UR	C5-C6-C7-C8
30	2	319	LHG	O1-C1-C2-O2
25	B	609	CLA	C2-C3-C5-C6
30	Y	318	LHG	C14-C15-C16-C17
24	R	608	CHL	C2C-C3C-CAC-CBC
32	d	409	SQD	C14-C15-C16-C17
33	D	401	LMG	C34-C35-C36-C37
33	i	101	LMG	C38-C39-C40-C41
24	Y	309	CHL	O1A-CGA-O2A-C1
24	g	310	CHL	CBD-CGD-O2D-CED
24	p	306	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	CBA-CGA-O2A-C1
24	G	313	CHL	CBA-CGA-O2A-C1
25	A	605	CLA	CBA-CGA-O2A-C1
29	9	301	0UR	C46-C47-C48-C49
24	Y	310	CHL	C4B-C3B-CAB-CBB
25	R	611	CLA	C4B-C3B-CAB-CBB
25	3	306	CLA	C4B-C3B-CAB-CBB
25	3	316	CLA	C4B-C3B-CAB-CBB
25	9	306	CLA	C4B-C3B-CAB-CBB
25	N	306	CLA	C4B-C3B-CAB-CBB
25	N	315	CLA	C4B-C3B-CAB-CBB
25	Y	315	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	8	305	CLA	C4B-C3B-CAB-CBB
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	616	CLA	C4B-C3B-CAB-CBB
25	A	605	CLA	C4B-C3B-CAB-CBB
25	6	306	CLA	C4B-C3B-CAB-CBB
25	6	307	CLA	C4B-C3B-CAB-CBB
25	g	316	CLA	C4B-C3B-CAB-CBB
25	u	307	CLA	C4B-C3B-CAB-CBB
25	n	306	CLA	C4B-C3B-CAB-CBB
25	y	316	CLA	C4B-C3B-CAB-CBB
25	q	305	CLA	C4B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4B-C3B-CAB-CBB
25	r	312	CLA	C4B-C3B-CAB-CBB
25	Y	316	CLA	C2A-CAA-CBA-CGA
25	p	308	CLA	C2A-CAA-CBA-CGA
37	c	619	DGD	O6E-C1E-O5D-C6D
29	7	301	0UR	C3-C4-C5-C6
31	C	614	8CT	C16-C17-C18-C19
31	c	614	8CT	C16-C17-C18-C19
24	R	607	CHL	O1A-CGA-O2A-C1
24	p	313	CHL	C2C-C3C-CAC-CBC
25	B	606	CLA	C15-C16-C17-C18
30	d	408	LHG	C28-C29-C30-C31
32	A	609	SQD	C13-C14-C15-C16
33	d	401	LMG	C18-C19-C20-C21
25	c	603	CLA	C5-C6-C7-C8
25	s	413	CLA	C2-C3-C5-C6
25	9	316	CLA	C11-C10-C8-C7
24	7	313	CHL	C2C-C3C-CAC-CBC
25	c	612	CLA	O1D-CGD-O2D-CED
24	Y	319	CHL	C2-C1-O2A-CGA
24	y	311	CHL	C2-C1-O2A-CGA
24	y	313	CHL	C2-C1-O2A-CGA
24	q	309	CHL	C2-C1-O2A-CGA
24	7	306	CHL	C2-C1-O2A-CGA
25	g	308	CLA	C2-C1-O2A-CGA
24	6	310	CHL	O1D-CGD-O2D-CED
25	B	607	CLA	C16-C17-C18-C20
25	7	314	CLA	C6-C7-C8-C9
32	d	409	SQD	C7-C8-C9-C10
25	c	602	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	3	304	CHL	C2A-CAA-CBA-CGA
24	N	310	CHL	C2A-CAA-CBA-CGA
24	n	310	CHL	C2A-CAA-CBA-CGA
25	N	313	CLA	C2A-CAA-CBA-CGA
25	Y	313	CLA	C2A-CAA-CBA-CGA
25	C	607	CLA	C2A-CAA-CBA-CGA
25	g	307	CLA	C2A-CAA-CBA-CGA
25	y	314	CLA	C2A-CAA-CBA-CGA
25	y	317	CLA	C2A-CAA-CBA-CGA
25	c	607	CLA	C2A-CAA-CBA-CGA
25	s	410	CLA	C2A-CAA-CBA-CGA
25	N	306	CLA	C6-C7-C8-C9
24	q	311	CHL	C4C-C3C-CAC-CBC
24	G	311	CHL	CAA-CBA-CGA-O1A
24	9	309	CHL	C3A-C2A-CAA-CBA
25	6	316	CLA	C3A-C2A-CAA-CBA
25	u	315	CLA	C3A-C2A-CAA-CBA
24	s	409	CHL	O1D-CGD-O2D-CED
24	8	310	CHL	C4C-C3C-CAC-CBC
25	a	605	CLA	O2A-C1-C2-C3
30	5	319	LHG	O8-C23-C24-C25
25	y	317	CLA	CBA-CGA-O2A-C1
25	q	306	CLA	CBA-CGA-O2A-C1
25	a	605	CLA	CBA-CGA-O2A-C1
25	R	611	CLA	CAA-CBA-CGA-O2A
25	g	316	CLA	CAA-CBA-CGA-O1A
39	d	406	PL9	C15-C14-C16-C17
30	9	318	LHG	C30-C31-C32-C33
33	d	401	LMG	C40-C41-C42-C43
30	9	318	LHG	O8-C23-C24-C25
24	S	602	CHL	C6-C7-C8-C9
24	g	313	CHL	C11-C10-C8-C9
24	u	305	CHL	C14-C13-C15-C16
24	p	305	CHL	C11-C10-C8-C9
24	s	403	CHL	C6-C7-C8-C9
24	7	305	CHL	C11-C10-C8-C9
24	7	306	CHL	C11-C10-C8-C9
25	Y	314	CLA	C6-C7-C8-C9
25	Y	314	CLA	C11-C12-C13-C14
25	Y	314	CLA	C14-C13-C15-C16
25	u	315	CLA	C6-C7-C8-C9
25	b	606	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	601	CLA	C11-C12-C13-C14
35	A	606	PHO	C6-C7-C8-C9
35	D	403	PHO	C6-C7-C8-C9
35	D	403	PHO	C11-C12-C13-C14
35	a	606	PHO	C6-C7-C8-C9
35	d	403	PHO	C6-C7-C8-C9
23	f	201	HEM	C3D-CAD-CBD-CGD
30	5	319	LHG	C9-C10-C11-C12
33	m	101	LMG	C11-C12-C13-C14
25	B	612	CLA	C13-C15-C16-C17
25	Y	316	CLA	CBA-CGA-O2A-C1
32	d	409	SQD	C27-C28-C29-C30
33	d	401	LMG	C36-C37-C38-C39
28	R	616	NEX	C39-C29-C30-C31
28	1	303	NEX	C39-C29-C30-C31
28	2	304	NEX	C39-C29-C30-C31
28	3	318	NEX	C39-C29-C30-C31
28	S	617	NEX	C39-C29-C30-C31
28	G	304	NEX	C39-C29-C30-C31
28	9	319	NEX	C39-C29-C30-C31
28	N	303	NEX	C39-C29-C30-C31
28	4	303	NEX	C39-C29-C30-C31
28	5	304	NEX	C39-C29-C30-C31
28	6	303	NEX	C39-C29-C30-C31
28	g	304	NEX	C39-C29-C30-C31
28	u	304	NEX	C39-C29-C30-C31
28	n	303	NEX	C39-C29-C30-C31
28	y	304	NEX	C39-C29-C30-C31
28	p	304	NEX	C39-C29-C30-C31
28	s	401	NEX	C39-C29-C30-C31
28	r	301	NEX	C39-C29-C30-C31
28	r	317	NEX	C39-C29-C30-C31
28	7	304	NEX	C39-C29-C30-C31
31	S	614	8CT	C40-C12-C13-C14
31	S	614	8CT	C39-C16-C17-C18
31	S	615	8CT	C39-C16-C17-C18
31	S	615	8CT	C19-C20-C21-C22
31	S	615	8CT	C24-C25-C26-C27
31	s	415	8CT	C40-C12-C13-C14
31	s	415	8CT	C39-C16-C17-C18
31	s	416	8CT	C39-C16-C17-C18
31	s	416	8CT	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	s	416	8CT	C24-C25-C26-C27
33	i	101	LMG	C7-C8-C9-O8
24	G	311	CHL	C3-C5-C6-C7
30	1	318	LHG	C27-C28-C29-C30
30	2	319	LHG	O8-C23-C24-C25
32	B	618	SQD	C16-C17-C18-C19
25	q	305	CLA	O1D-CGD-O2D-CED
33	d	411	LMG	C30-C31-C32-C33
25	8	306	CLA	CBA-CGA-O2A-C1
37	C	620	DGD	O6E-C1E-O5D-C6D
30	g	319	LHG	C11-C10-C9-C8
24	u	310	CHL	CAA-CBA-CGA-O1A
25	G	316	CLA	CAA-CBA-CGA-O1A
25	9	315	CLA	CAA-CBA-CGA-O1A
24	6	310	CHL	CBD-CGD-O2D-CED
30	2	319	LHG	C9-C10-C11-C12
24	9	309	CHL	CAA-CBA-CGA-O1A
37	c	618	DGD	C1G-C2G-O2G-C1B
24	G	305	CHL	C4-C3-C5-C6
25	C	610	CLA	C4-C3-C5-C6
37	c	619	DGD	O6D-C5D-C6D-O5D
24	S	601	CHL	C1A-C2A-CAA-CBA
24	9	309	CHL	C1A-C2A-CAA-CBA
25	R	612	CLA	C1A-C2A-CAA-CBA
25	G	314	CLA	C1A-C2A-CAA-CBA
25	B	603	CLA	C1A-C2A-CAA-CBA
25	C	606	CLA	C1A-C2A-CAA-CBA
25	C	608	CLA	C1A-C2A-CAA-CBA
25	C	616	CLA	C1A-C2A-CAA-CBA
25	5	314	CLA	C1A-C2A-CAA-CBA
25	g	314	CLA	C1A-C2A-CAA-CBA
25	q	306	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	c	606	CLA	C1A-C2A-CAA-CBA
25	c	608	CLA	C1A-C2A-CAA-CBA
25	c	616	CLA	C1A-C2A-CAA-CBA
25	r	310	CLA	C1A-C2A-CAA-CBA
25	B	603	CLA	C11-C12-C13-C15
25	C	607	CLA	C6-C7-C8-C10
25	b	603	CLA	C11-C12-C13-C15
25	c	607	CLA	C6-C7-C8-C10
25	c	611	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	4	318	LHG	C11-C10-C9-C8
24	9	309	CHL	CAA-CBA-CGA-O2A
25	2	316	CLA	CAA-CBA-CGA-O1A
25	S	611	CLA	CAA-CBA-CGA-O1A
25	5	316	CLA	CAA-CBA-CGA-O1A
25	s	412	CLA	CAA-CBA-CGA-O1A
24	1	309	CHL	C3C-C2C-CMC-OMC
24	G	305	CHL	C3C-C2C-CMC-OMC
24	5	313	CHL	C3C-C2C-CMC-OMC
24	6	311	CHL	C3C-C2C-CMC-OMC
24	6	312	CHL	C3C-C2C-CMC-OMC
24	g	305	CHL	C3C-C2C-CMC-OMC
25	R	613	CLA	CAA-CBA-CGA-O2A
25	p	317	CLA	C11-C10-C8-C7
25	S	609	CLA	C2A-CAA-CBA-CGA
25	7	308	CLA	C2A-CAA-CBA-CGA
25	b	612	CLA	C13-C15-C16-C17
25	b	613	CLA	C5-C6-C7-C8
33	m	101	LMG	C30-C31-C32-C33
25	p	307	CLA	CBA-CGA-O2A-C1
24	S	608	CHL	CBD-CGD-O2D-CED
25	C	603	CLA	C5-C6-C7-C8
25	C	607	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
24	q	308	CHL	CAA-CBA-CGA-O1A
24	q	308	CHL	CAA-CBA-CGA-O2A
30	A	601	LHG	C26-C27-C28-C29
25	c	612	CLA	C4-C3-C5-C6
25	Y	314	CLA	C5-C6-C7-C8
25	C	610	CLA	C2-C3-C5-C6
24	9	305	CHL	C2B-C3B-CAB-CBB
24	N	305	CHL	C2B-C3B-CAB-CBB
24	Y	310	CHL	C2B-C3B-CAB-CBB
24	u	306	CHL	C2B-C3B-CAB-CBB
24	n	305	CHL	C2B-C3B-CAB-CBB
24	p	305	CHL	C2B-C3B-CAB-CBB
24	p	306	CHL	C2B-C3B-CAB-CBB
24	7	305	CHL	C2B-C3B-CAB-CBB
24	7	306	CHL	C2B-C3B-CAB-CBB
25	R	611	CLA	C2B-C3B-CAB-CBB
25	R	612	CLA	C2B-C3B-CAB-CBB
25	1	315	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	2	315	CLA	C2B-C3B-CAB-CBB
25	3	306	CLA	C2B-C3B-CAB-CBB
25	N	315	CLA	C2B-C3B-CAB-CBB
25	Y	315	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	616	CLA	C2B-C3B-CAB-CBB
25	C	602	CLA	C2B-C3B-CAB-CBB
25	5	315	CLA	C2B-C3B-CAB-CBB
25	6	306	CLA	C2B-C3B-CAB-CBB
25	6	307	CLA	C2B-C3B-CAB-CBB
25	6	316	CLA	C2B-C3B-CAB-CBB
25	n	315	CLA	C2B-C3B-CAB-CBB
25	y	316	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C2B-C3B-CAB-CBB
25	b	616	CLA	C2B-C3B-CAB-CBB
25	a	605	CLA	C2B-C3B-CAB-CBB
25	c	602	CLA	C2B-C3B-CAB-CBB
25	s	411	CLA	C2B-C3B-CAB-CBB
37	C	619	DGD	C5A-C6A-C7A-C8A
25	R	611	CLA	CAA-CBA-CGA-O1A
25	A	605	CLA	O1A-CGA-O2A-C1
25	B	613	CLA	C3-C5-C6-C7
33	m	101	LMG	O8-C28-C29-C30
37	C	619	DGD	C1A-C2A-C3A-C4A
24	5	305	CHL	C2C-C3C-CAC-CBC
30	1	318	LHG	C25-C26-C27-C28
28	R	616	NEX	C28-C29-C30-C31
28	1	303	NEX	C28-C29-C30-C31
28	2	304	NEX	C28-C29-C30-C31
28	3	318	NEX	C28-C29-C30-C31
28	S	617	NEX	C28-C29-C30-C31
28	G	304	NEX	C28-C29-C30-C31
28	9	319	NEX	C28-C29-C30-C31
28	N	303	NEX	C28-C29-C30-C31
28	4	303	NEX	C28-C29-C30-C31
28	5	304	NEX	C28-C29-C30-C31
28	6	303	NEX	C28-C29-C30-C31
28	g	304	NEX	C28-C29-C30-C31
28	u	304	NEX	C28-C29-C30-C31
28	n	303	NEX	C28-C29-C30-C31
28	y	304	NEX	C28-C29-C30-C31
28	p	304	NEX	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	s	401	NEX	C28-C29-C30-C31
28	r	301	NEX	C28-C29-C30-C31
28	r	317	NEX	C28-C29-C30-C31
28	7	304	NEX	C28-C29-C30-C31
31	S	614	8CT	C11-C12-C13-C14
31	S	614	8CT	C15-C16-C17-C18
31	S	615	8CT	C15-C16-C17-C18
31	S	615	8CT	C24-C25-C26-C28
31	s	415	8CT	C11-C12-C13-C14
31	s	415	8CT	C15-C16-C17-C18
31	s	416	8CT	C15-C16-C17-C18
31	s	416	8CT	C24-C25-C26-C28
25	B	613	CLA	C5-C6-C7-C8
24	8	308	CHL	CAA-CBA-CGA-O2A
25	n	315	CLA	CAA-CBA-CGA-O1A
24	p	306	CHL	O1D-CGD-O2D-CED
30	A	612	LHG	O7-C5-C6-O8
30	a	612	LHG	O7-C5-C6-O8
33	C	618	LMG	C17-C18-C19-C20
24	4	308	CHL	O1D-CGD-O2D-CED
24	6	304	CHL	C2A-CAA-CBA-CGA
25	2	317	CLA	C2A-CAA-CBA-CGA
30	a	601	LHG	C19-C20-C21-C22
31	D	410	8CT	C18-C19-C20-C21
24	8	308	CHL	CAA-CBA-CGA-O1A
24	6	310	CHL	CAA-CBA-CGA-O2A
24	r	309	CHL	CAA-CBA-CGA-O1A
25	r	312	CLA	CAA-CBA-CGA-O1A
25	q	306	CLA	O1A-CGA-O2A-C1
25	B	602	CLA	C13-C15-C16-C17
30	n	318	LHG	C27-C28-C29-C30
24	G	313	CHL	O1A-CGA-O2A-C1
25	a	605	CLA	O1A-CGA-O2A-C1
24	r	309	CHL	CAA-CBA-CGA-O2A
25	2	316	CLA	CAA-CBA-CGA-O2A
25	S	611	CLA	CAA-CBA-CGA-O2A
25	G	316	CLA	CAA-CBA-CGA-O2A
25	N	315	CLA	CAA-CBA-CGA-O1A
25	s	412	CLA	CAA-CBA-CGA-O2A
33	i	101	LMG	C14-C15-C16-C17
25	8	305	CLA	O1D-CGD-O2D-CED
25	A	607	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	607	CLA	C4-C3-C5-C6
24	3	309	CHL	C2-C1-O2A-CGA
24	G	306	CHL	C2-C1-O2A-CGA
24	N	310	CHL	C2-C1-O2A-CGA
24	g	306	CHL	C2-C1-O2A-CGA
24	n	310	CHL	C2-C1-O2A-CGA
24	q	304	CHL	C2-C1-O2A-CGA
25	C	612	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
25	8	306	CLA	O1A-CGA-O2A-C1
25	y	317	CLA	O1A-CGA-O2A-C1
24	u	310	CHL	CAA-CBA-CGA-O2A
25	5	316	CLA	CAA-CBA-CGA-O2A
25	q	314	CLA	CAA-CBA-CGA-O2A
30	y	319	LHG	C29-C30-C31-C32
24	r	307	CHL	CAA-CBA-CGA-O2A
25	r	314	CLA	CAA-CBA-CGA-O2A
30	G	319	LHG	O8-C23-C24-C25
24	G	313	CHL	C11-C10-C8-C9
24	p	306	CHL	C11-C10-C8-C9
25	N	314	CLA	C6-C7-C8-C9
24	y	310	CHL	O1A-CGA-O2A-C1
25	Y	316	CLA	O1A-CGA-O2A-C1
25	p	307	CLA	O1A-CGA-O2A-C1
24	R	608	CHL	CAA-CBA-CGA-O2A
25	9	315	CLA	CAA-CBA-CGA-O2A
25	y	316	CLA	CAA-CBA-CGA-O2A
30	c	617	LHG	O8-C23-C24-C25
30	a	601	LHG	C16-C17-C18-C19
37	C	620	DGD	C4A-C5A-C6A-C7A
25	R	613	CLA	C2A-CAA-CBA-CGA
25	5	317	CLA	C2A-CAA-CBA-CGA
25	r	314	CLA	C2A-CAA-CBA-CGA
25	g	316	CLA	CAA-CBA-CGA-O2A
30	d	408	LHG	C10-C11-C12-C13
31	V	401	8CT	C04-C03-C10-C11
31	v	401	8CT	C04-C03-C10-C11
30	C	617	LHG	O8-C23-C24-C25
30	p	319	LHG	C9-C10-C11-C12
24	3	310	CHL	CAA-CBA-CGA-O2A
25	6	316	CLA	CAA-CBA-CGA-O2A
25	u	316	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	n	315	CLA	CAA-CBA-CGA-O2A
25	c	607	CLA	C13-C15-C16-C17
31	C	614	8CT	C23-C24-C25-C26
31	D	410	8CT	C12-C13-C14-C15
30	A	601	LHG	C19-C20-C21-C22
33	i	101	LMG	C13-C14-C15-C16
24	G	306	CHL	C4-C3-C5-C6
24	Y	319	CHL	C4-C3-C5-C6
24	8	310	CHL	C4-C3-C5-C6
24	g	305	CHL	C4-C3-C5-C6
24	q	309	CHL	C4-C3-C5-C6
25	C	604	CLA	C4-C3-C5-C6
25	c	604	CLA	C4-C3-C5-C6
28	1	303	NEX	C31-C32-C33-C34
28	2	304	NEX	C31-C32-C33-C34
28	S	617	NEX	C31-C32-C33-C34
28	9	319	NEX	C31-C32-C33-C34
28	4	303	NEX	C31-C32-C33-C34
28	5	304	NEX	C31-C32-C33-C34
28	u	304	NEX	C31-C32-C33-C34
28	y	304	NEX	C31-C32-C33-C34
28	p	304	NEX	C31-C32-C33-C34
28	7	304	NEX	C31-C32-C33-C34
29	3	301	0UR	C5-C6-C7-C8
25	C	604	CLA	C10-C11-C12-C13
25	C	609	CLA	C10-C11-C12-C13
25	c	609	CLA	C10-C11-C12-C13
24	Y	312	CHL	C2-C3-C5-C6
30	g	319	LHG	O8-C23-C24-C25
25	R	612	CLA	CAA-CBA-CGA-O2A
25	y	316	CLA	CAA-CBA-CGA-O1A
24	R	607	CHL	C2-C1-O2A-CGA
24	G	313	CHL	C4C-C3C-CAC-CBC
30	A	601	LHG	C16-C17-C18-C19
24	S	601	CHL	CAA-CBA-CGA-O2A
25	N	315	CLA	CAA-CBA-CGA-O2A
25	Y	315	CLA	CAA-CBA-CGA-O1A
25	Y	315	CLA	CAA-CBA-CGA-O2A
25	8	313	CLA	CAA-CBA-CGA-O2A
25	r	312	CLA	CAA-CBA-CGA-O2A
30	1	318	LHG	C9-C10-C11-C12
32	A	609	SQD	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	N	313	CLA	C6-C7-C8-C10
30	A	601	LHG	O6-C4-C5-O7
25	C	608	CLA	C14-C13-C15-C16
33	B	619	LMG	C30-C31-C32-C33
24	R	608	CHL	CAA-CBA-CGA-O1A
24	p	310	CHL	CAA-CBA-CGA-O2A
24	7	310	CHL	CAA-CBA-CGA-O2A
25	1	315	CLA	CAA-CBA-CGA-O2A
25	8	313	CLA	CAA-CBA-CGA-O1A
25	4	315	CLA	CAA-CBA-CGA-O2A
25	6	316	CLA	CAA-CBA-CGA-O1A
25	4	313	CLA	C2A-CAA-CBA-CGA
24	N	309	CHL	CBD-CGD-O2D-CED
25	7	314	CLA	O1A-CGA-O2A-C1
24	6	310	CHL	CAA-CBA-CGA-O1A
24	s	402	CHL	CAA-CBA-CGA-O2A
25	u	316	CLA	CAA-CBA-CGA-O1A
25	p	316	CLA	CAA-CBA-CGA-O1A
25	q	314	CLA	CAA-CBA-CGA-O1A
25	7	316	CLA	CAA-CBA-CGA-O1A
25	R	604	CLA	O1D-CGD-O2D-CED
25	G	316	CLA	C4B-C3B-CAB-CBB
25	C	602	CLA	C4B-C3B-CAB-CBB
25	n	315	CLA	C4B-C3B-CAB-CBB
25	a	605	CLA	C4B-C3B-CAB-CBB
25	c	602	CLA	C4B-C3B-CAB-CBB
25	s	411	CLA	C4B-C3B-CAB-CBB
25	n	313	CLA	C6-C7-C8-C10
24	2	305	CHL	C2C-C3C-CAC-CBC
30	p	319	LHG	C26-C27-C28-C29
30	A	601	LHG	O6-C4-C5-C6
24	N	310	CHL	CAA-CBA-CGA-O2A
24	n	310	CHL	CAA-CBA-CGA-O2A
25	8	312	CLA	O1A-CGA-O2A-C1
25	p	314	CLA	O1A-CGA-O2A-C1
24	q	311	CHL	C4-C3-C5-C6
24	G	305	CHL	C11-C12-C13-C15
24	G	313	CHL	C11-C12-C13-C15
24	n	305	CHL	C11-C10-C8-C7
25	G	315	CLA	C11-C10-C8-C7
25	N	314	CLA	C6-C7-C8-C10
25	Y	314	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	Y	316	CLA	C2-C3-C5-C6
25	C	602	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C10-C8-C7
25	b	605	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
25	7	317	CLA	C2-C3-C5-C6
25	s	404	CLA	CAA-CBA-CGA-O2A
24	g	313	CHL	CBA-CGA-O2A-C1
25	b	609	CLA	C13-C15-C16-C17
24	r	308	CHL	C2-C1-O2A-CGA
31	c	614	8CT	C23-C24-C25-C26
32	B	618	SQD	C2-C1-O6-C44
24	8	310	CHL	C6-C7-C8-C10
25	7	314	CLA	C6-C7-C8-C10
24	1	312	CHL	CAA-CBA-CGA-O2A
24	4	312	CHL	CAA-CBA-CGA-O2A
25	p	316	CLA	CAA-CBA-CGA-O2A
24	3	304	CHL	C2-C1-O2A-CGA
24	6	304	CHL	C2-C1-O2A-CGA
30	9	318	LHG	C9-C10-C11-C12
30	n	318	LHG	O10-C23-C24-C25
25	R	604	CLA	CBD-CGD-O2D-CED
30	d	408	LHG	C32-C33-C34-C35
25	1	315	CLA	CAA-CBA-CGA-O1A
25	3	316	CLA	CAA-CBA-CGA-O2A
25	4	315	CLA	CAA-CBA-CGA-O1A
24	N	311	CHL	O2A-C1-C2-C3
24	8	309	CHL	O2A-C1-C2-C3
24	n	311	CHL	O2A-C1-C2-C3
24	q	310	CHL	O2A-C1-C2-C3
30	y	319	LHG	O8-C23-C24-C25
30	Y	318	LHG	C29-C30-C31-C32
25	3	315	CLA	CAA-CBA-CGA-O2A
25	S	616	CLA	CAA-CBA-CGA-O2A
25	7	316	CLA	CAA-CBA-CGA-O2A
25	8	312	CLA	CBA-CGA-O2A-C1
25	7	307	CLA	CBA-CGA-O2A-C1
25	7	314	CLA	CBA-CGA-O2A-C1
29	N	301	0UR	O42-C2-C3-C4
29	n	301	0UR	O42-C2-C3-C4
29	p	301	0UR	O42-C2-C3-C4
29	7	301	0UR	O42-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	n	305	CHL	C4-C3-C5-C6
24	s	403	CHL	C4-C3-C5-C6
25	C	605	CLA	C4-C3-C5-C6
25	c	605	CLA	C4-C3-C5-C6
39	D	406	PL9	C15-C14-C16-C17
39	D	406	PL9	C40-C39-C41-C42
25	b	602	CLA	C5-C6-C7-C8
25	2	307	CLA	C2A-CAA-CBA-CGA
24	n	309	CHL	CAA-CBA-CGA-O2A
25	6	315	CLA	CAA-CBA-CGA-O2A
25	B	605	CLA	C2-C3-C5-C6
25	C	604	CLA	C2-C3-C5-C6
24	r	309	CHL	C4C-C3C-CAC-CBC
24	Y	305	CHL	CAA-CBA-CGA-O2A
24	G	305	CHL	C6-C7-C8-C9
24	G	305	CHL	C11-C12-C13-C14
24	g	305	CHL	C6-C7-C8-C9
25	9	314	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C10-C8-C9
25	C	604	CLA	C6-C7-C8-C9
25	C	608	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	n	314	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C12-C13-C14
24	g	313	CHL	O1A-CGA-O2A-C1
24	R	608	CHL	C4C-C3C-CAC-CBC
25	S	603	CLA	CAA-CBA-CGA-O2A
37	c	619	DGD	CBB-CCB-CDB-CEB
24	N	304	CHL	C3A-C2A-CAA-CBA
24	u	305	CHL	C3A-C2A-CAA-CBA
24	n	304	CHL	C3A-C2A-CAA-CBA
25	9	314	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	n	316	CLA	C3A-C2A-CAA-CBA
25	d	404	CLA	C3A-C2A-CAA-CBA
25	C	602	CLA	O1A-CGA-O2A-C1
24	p	310	CHL	CAA-CBA-CGA-O1A
24	7	310	CHL	CAA-CBA-CGA-O1A
24	5	306	CHL	O1A-CGA-O2A-C1
24	R	607	CHL	CAD-CBD-CGD-O2D
24	2	318	CHL	CAD-CBD-CGD-O2D
24	9	317	CHL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	4	317	CHL	CAD-CBD-CGD-O2D
24	5	318	CHL	CAD-CBD-CGD-O2D
24	u	318	CHL	CAD-CBD-CGD-O2D
25	R	604	CLA	CAD-CBD-CGD-O2D
25	1	306	CLA	CAD-CBD-CGD-O2D
25	1	313	CLA	CAD-CBD-CGD-O2D
25	2	314	CLA	CAD-CBD-CGD-O2D
25	9	307	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	A	603	CLA	CAD-CBD-CGD-O2D
25	C	601	CLA	CAD-CBD-CGD-O2D
25	C	606	CLA	CAD-CBD-CGD-O2D
25	C	610	CLA	CAD-CBD-CGD-O2D
25	D	404	CLA	CAD-CBD-CGD-O2D
25	4	306	CLA	CAD-CBD-CGD-O2D
25	4	313	CLA	CAD-CBD-CGD-O2D
25	5	314	CLA	CAD-CBD-CGD-O2D
25	u	308	CLA	CAD-CBD-CGD-O2D
25	p	314	CLA	CAD-CBD-CGD-O2D
25	q	312	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	a	603	CLA	CAD-CBD-CGD-O2D
25	c	601	CLA	CAD-CBD-CGD-O2D
25	c	606	CLA	CAD-CBD-CGD-O2D
25	c	610	CLA	CAD-CBD-CGD-O2D
25	r	305	CLA	CAD-CBD-CGD-O2D
25	7	314	CLA	CAD-CBD-CGD-O2D
35	A	606	PHO	CAD-CBD-CGD-O2D
35	D	403	PHO	CAD-CBD-CGD-O2D
35	a	606	PHO	CAD-CBD-CGD-O2D
35	d	403	PHO	CAD-CBD-CGD-O2D
37	C	619	DGD	C1G-C2G-O2G-C1B
37	c	618	DGD	C3G-C2G-O2G-C1B
30	p	319	LHG	C7-C8-C9-C10
25	B	607	CLA	C16-C17-C18-C19
30	4	318	LHG	C9-C10-C11-C12
29	Y	301	0UR	C3-C4-C5-C6
25	9	306	CLA	C2A-CAA-CBA-CGA
25	u	307	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1	305	CHL	CAA-CBA-CGA-O2A
24	S	601	CHL	CAA-CBA-CGA-O1A
24	N	309	CHL	CAA-CBA-CGA-O2A
25	s	417	CLA	CAA-CBA-CGA-O2A
24	q	309	CHL	CBD-CGD-O2D-CED
24	S	602	CHL	C4-C3-C5-C6
24	q	311	CHL	C6-C7-C8-C10
24	p	306	CHL	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
24	2	312	CHL	CAA-CBA-CGA-O2A
25	c	612	CLA	C2-C3-C5-C6
24	y	306	CHL	CAA-CBA-CGA-O2A
25	B	606	CLA	CAA-CBA-CGA-O2A
33	D	411	LMG	O7-C10-C11-C12
37	C	620	DGD	O2G-C1B-C2B-C3B
28	R	616	NEX	C31-C32-C33-C34
28	G	304	NEX	C31-C32-C33-C34
28	g	304	NEX	C31-C32-C33-C34
28	r	317	NEX	C31-C32-C33-C34
25	5	307	CLA	C2A-CAA-CBA-CGA
30	1	318	LHG	C2-C3-O3-P
24	1	312	CHL	CAA-CBA-CGA-O1A
24	s	402	CHL	CAA-CBA-CGA-O1A
25	p	314	CLA	CBA-CGA-O2A-C1
25	7	307	CLA	O1A-CGA-O2A-C1
30	2	319	LHG	O6-C4-C5-O7
30	5	319	LHG	O6-C4-C5-O7
25	C	603	CLA	C10-C11-C12-C13
25	g	317	CLA	C11-C10-C8-C7
30	9	318	LHG	C23-C24-C25-C26
25	A	605	CLA	O2A-C1-C2-C3
24	Y	310	CHL	CAA-CBA-CGA-O1A
24	2	312	CHL	CAA-CBA-CGA-O1A
24	3	310	CHL	CAA-CBA-CGA-O1A
24	5	312	CHL	CAA-CBA-CGA-O2A
25	r	313	CLA	CAA-CBA-CGA-O2A
24	R	606	CHL	C2-C1-O2A-CGA
33	D	411	LMG	C21-C22-C23-C24
24	N	304	CHL	O2A-C1-C2-C3
24	Y	312	CHL	O2A-C1-C2-C3
24	g	312	CHL	O2A-C1-C2-C3
24	n	304	CHL	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	n	312	CHL	O2A-C1-C2-C3
24	y	313	CHL	O2A-C1-C2-C3
25	G	307	CLA	O2A-C1-C2-C3
25	N	306	CLA	O2A-C1-C2-C3
25	8	305	CLA	O2A-C1-C2-C3
25	B	614	CLA	O2A-C1-C2-C3
25	C	609	CLA	O2A-C1-C2-C3
25	D	404	CLA	O2A-C1-C2-C3
25	g	307	CLA	O2A-C1-C2-C3
25	p	315	CLA	O2A-C1-C2-C3
25	q	305	CLA	O2A-C1-C2-C3
25	b	614	CLA	O2A-C1-C2-C3
25	c	609	CLA	O2A-C1-C2-C3
25	d	404	CLA	O2A-C1-C2-C3
25	7	315	CLA	O2A-C1-C2-C3
35	A	606	PHO	O2A-C1-C2-C3
35	D	403	PHO	O2A-C1-C2-C3
25	B	612	CLA	CBA-CGA-O2A-C1
25	1	313	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	CAA-CBA-CGA-O2A
24	S	605	CHL	CAA-CBA-CGA-O2A
24	N	309	CHL	CAA-CBA-CGA-O1A
24	4	312	CHL	CAA-CBA-CGA-O1A
25	R	612	CLA	CAA-CBA-CGA-O1A
25	S	616	CLA	CAA-CBA-CGA-O1A
25	s	404	CLA	CAA-CBA-CGA-O1A
24	q	304	CHL	C10-C11-C12-C13
30	a	612	LHG	C13-C14-C15-C16
24	2	306	CHL	O1A-CGA-O2A-C1
24	s	409	CHL	CBD-CGD-O2D-CED
24	7	306	CHL	CBD-CGD-O2D-CED
33	w	201	LMG	C11-C12-C13-C14
33	d	401	LMG	C39-C40-C41-C42
24	G	305	CHL	CHA-CBD-CGD-O1D
24	G	305	CHL	CHA-CBD-CGD-O2D
24	G	313	CHL	CHA-CBD-CGD-O1D
24	G	313	CHL	CHA-CBD-CGD-O2D
24	9	312	CHL	CHA-CBD-CGD-O1D
24	9	312	CHL	CHA-CBD-CGD-O2D
24	g	305	CHL	CHA-CBD-CGD-O1D
24	g	305	CHL	CHA-CBD-CGD-O2D
24	u	313	CHL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	u	313	CHL	CHA-CBD-CGD-O2D
24	n	308	CHL	CHA-CBD-CGD-O1D
24	n	308	CHL	CHA-CBD-CGD-O2D
25	R	610	CLA	CHA-CBD-CGD-O1D
25	R	610	CLA	CHA-CBD-CGD-O2D
25	R	611	CLA	CHA-CBD-CGD-O1D
25	R	611	CLA	CHA-CBD-CGD-O2D
25	1	307	CLA	CHA-CBD-CGD-O1D
25	1	307	CLA	CHA-CBD-CGD-O2D
25	3	306	CLA	CHA-CBD-CGD-O1D
25	3	307	CLA	CHA-CBD-CGD-O1D
25	3	307	CLA	CHA-CBD-CGD-O2D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	G	307	CLA	CHA-CBD-CGD-O1D
25	G	307	CLA	CHA-CBD-CGD-O2D
25	G	308	CLA	CHA-CBD-CGD-O1D
25	G	308	CLA	CHA-CBD-CGD-O2D
25	G	316	CLA	CHA-CBD-CGD-O1D
25	G	316	CLA	CHA-CBD-CGD-O2D
25	9	315	CLA	CHA-CBD-CGD-O2D
25	N	314	CLA	CHA-CBD-CGD-O1D
25	N	314	CLA	CHA-CBD-CGD-O2D
25	N	315	CLA	CHA-CBD-CGD-O1D
25	Y	316	CLA	CHA-CBD-CGD-O1D
25	Y	316	CLA	CHA-CBD-CGD-O2D
25	8	306	CLA	CHA-CBD-CGD-O2D
25	B	604	CLA	CHA-CBD-CGD-O1D
25	C	607	CLA	CHA-CBD-CGD-O2D
25	C	616	CLA	CHA-CBD-CGD-O1D
25	C	616	CLA	CHA-CBD-CGD-O2D
25	4	307	CLA	CHA-CBD-CGD-O1D
25	4	307	CLA	CHA-CBD-CGD-O2D
25	5	307	CLA	CHA-CBD-CGD-O2D
25	6	306	CLA	CHA-CBD-CGD-O1D
25	6	307	CLA	CHA-CBD-CGD-O1D
25	6	307	CLA	CHA-CBD-CGD-O2D
25	6	315	CLA	CHA-CBD-CGD-O2D
25	g	307	CLA	CHA-CBD-CGD-O1D
25	g	307	CLA	CHA-CBD-CGD-O2D
25	g	308	CLA	CHA-CBD-CGD-O1D
25	g	308	CLA	CHA-CBD-CGD-O2D
25	g	316	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	n	314	CLA	CHA-CBD-CGD-O1D
25	n	314	CLA	CHA-CBD-CGD-O2D
25	y	308	CLA	CHA-CBD-CGD-O1D
25	y	308	CLA	CHA-CBD-CGD-O2D
25	y	317	CLA	CHA-CBD-CGD-O1D
25	y	317	CLA	CHA-CBD-CGD-O2D
25	p	308	CLA	CHA-CBD-CGD-O2D
25	p	315	CLA	CHA-CBD-CGD-O1D
25	p	315	CLA	CHA-CBD-CGD-O2D
25	p	317	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	CHA-CBD-CGD-O1D
25	c	607	CLA	CHA-CBD-CGD-O1D
25	c	607	CLA	CHA-CBD-CGD-O2D
25	c	616	CLA	CHA-CBD-CGD-O1D
25	c	616	CLA	CHA-CBD-CGD-O2D
25	s	404	CLA	CHA-CBD-CGD-O2D
25	s	405	CLA	CHA-CBD-CGD-O2D
25	r	311	CLA	CHA-CBD-CGD-O1D
25	r	311	CLA	CHA-CBD-CGD-O2D
25	r	312	CLA	CHA-CBD-CGD-O2D
25	7	308	CLA	CHA-CBD-CGD-O2D
25	7	315	CLA	CHA-CBD-CGD-O2D
25	S	603	CLA	CAA-CBA-CGA-O1A
25	r	313	CLA	CAA-CBA-CGA-O1A
39	d	406	PL9	C40-C39-C41-C42
25	b	606	CLA	CAA-CBA-CGA-O2A
24	s	403	CHL	C2-C3-C5-C6
25	y	317	CLA	C2-C3-C5-C6
25	c	604	CLA	C2-C3-C5-C6
30	N	318	LHG	C27-C28-C29-C30
24	4	305	CHL	CAA-CBA-CGA-O2A
24	5	312	CHL	CAA-CBA-CGA-O1A
24	s	406	CHL	CAA-CBA-CGA-O2A
25	6	315	CLA	CAA-CBA-CGA-O1A
25	r	311	CLA	CAA-CBA-CGA-O2A
30	A	601	LHG	C9-C10-C11-C12
30	d	407	LHG	O7-C7-C8-C9
24	3	312	CHL	C2C-C3C-CAC-CBC
30	D	407	LHG	C11-C12-C13-C14
32	a	609	SQD	O47-C45-C46-O48
37	c	618	DGD	C1A-C2A-C3A-C4A
24	7	306	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	y	311	CHL	C5-C6-C7-C8
30	7	319	LHG	C26-C27-C28-C29
33	m	101	LMG	C16-C17-C18-C19
24	1	305	CHL	CAA-CBA-CGA-O1A
25	s	417	CLA	CAA-CBA-CGA-O1A
24	p	313	CHL	C4C-C3C-CAC-CBC
24	7	313	CHL	C4C-C3C-CAC-CBC
25	c	602	CLA	O1A-CGA-O2A-C1
25	C	601	CLA	CAA-CBA-CGA-O2A
25	c	601	CLA	CAA-CBA-CGA-O2A
30	N	318	LHG	O10-C23-C24-C25
30	a	601	LHG	C26-C27-C28-C29
25	b	612	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	CAA-CBA-CGA-O2A
25	C	612	CLA	C4-C3-C5-C6
24	Y	305	CHL	C6-C7-C8-C10
24	Y	312	CHL	C6-C7-C8-C10
24	g	305	CHL	C11-C12-C13-C15
24	y	306	CHL	C11-C12-C13-C15
24	y	313	CHL	C6-C7-C8-C10
25	C	604	CLA	C12-C13-C15-C16
25	y	315	CLA	C12-C13-C15-C16
25	b	607	CLA	C16-C17-C18-C20
30	Y	318	LHG	O8-C23-C24-C25
30	D	407	LHG	O7-C7-C8-C9
30	D	407	LHG	C33-C34-C35-C36
24	Y	304	CHL	C6-C7-C8-C9
25	B	605	CLA	C11-C12-C13-C14
25	C	602	CLA	C11-C12-C13-C14
25	C	607	CLA	C6-C7-C8-C9
25	c	604	CLA	C6-C7-C8-C9
25	c	607	CLA	C6-C7-C8-C9
39	D	406	PL9	C34-C36-C37-C38
24	5	310	CHL	C2B-C3B-CAB-CBB
25	G	316	CLA	C2B-C3B-CAB-CBB
25	A	603	CLA	C2B-C3B-CAB-CBB
25	C	603	CLA	C2B-C3B-CAB-CBB
25	a	603	CLA	C2B-C3B-CAB-CBB
30	7	319	LHG	C7-C8-C9-C10
25	C	602	CLA	CBA-CGA-O2A-C1
26	3	302	0IE	O29-C20-C3-C4
26	9	302	0IE	O29-C20-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	6	302	0IE	O29-C20-C3-C4
26	u	302	0IE	O29-C20-C3-C4
26	u	303	0IE	O29-C20-C3-C4
26	p	302	0IE	O29-C20-C3-C4
26	p	303	0IE	O29-C20-C3-C4
26	7	302	0IE	O29-C20-C3-C4
32	a	609	SQD	C4-C5-C6-S
24	n	305	CHL	C10-C11-C12-C13
24	Y	310	CHL	C5-C6-C7-C8
24	n	309	CHL	CAA-CBA-CGA-O1A
25	3	315	CLA	CAA-CBA-CGA-O1A
25	3	316	CLA	CAA-CBA-CGA-O1A
25	N	314	CLA	C2A-CAA-CBA-CGA
33	D	411	LMG	O9-C10-C11-C12
37	C	620	DGD	O1B-C1B-C2B-C3B
25	c	603	CLA	C10-C11-C12-C13
24	N	305	CHL	C11-C12-C13-C14
30	Y	318	LHG	C28-C29-C30-C31
24	g	306	CHL	C4-C3-C5-C6
25	7	317	CLA	C4-C3-C5-C6
30	5	319	LHG	O1-C1-C2-C3
24	9	304	CHL	O1A-CGA-O2A-C1
30	5	319	LHG	C25-C26-C27-C28
30	y	319	LHG	C28-C29-C30-C31
33	i	101	LMG	C32-C33-C34-C35
28	3	318	NEX	C11-C12-C13-C14
28	N	303	NEX	C11-C12-C13-C14
28	6	303	NEX	C11-C12-C13-C14
28	n	303	NEX	C11-C12-C13-C14
28	s	401	NEX	C11-C12-C13-C14
28	r	301	NEX	C11-C12-C13-C14
24	9	304	CHL	CBA-CGA-O2A-C1
25	G	317	CLA	CBA-CGA-O2A-C1
25	c	602	CLA	CBA-CGA-O2A-C1
24	2	311	CHL	C1A-C2A-CAA-CBA
24	9	304	CHL	C1A-C2A-CAA-CBA
24	N	304	CHL	C1A-C2A-CAA-CBA
24	5	311	CHL	C1A-C2A-CAA-CBA
24	u	305	CHL	C1A-C2A-CAA-CBA
24	n	304	CHL	C1A-C2A-CAA-CBA
25	R	609	CLA	C1A-C2A-CAA-CBA
25	2	307	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	2	314	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	C1A-C2A-CAA-CBA
25	9	314	CLA	C1A-C2A-CAA-CBA
25	Y	313	CLA	C1A-C2A-CAA-CBA
25	8	305	CLA	C1A-C2A-CAA-CBA
25	B	608	CLA	C1A-C2A-CAA-CBA
25	5	307	CLA	C1A-C2A-CAA-CBA
25	6	316	CLA	C1A-C2A-CAA-CBA
25	u	315	CLA	C1A-C2A-CAA-CBA
25	n	316	CLA	C1A-C2A-CAA-CBA
25	y	314	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C1A-C2A-CAA-CBA
25	4	313	CLA	C6-C7-C8-C10
32	a	609	SQD	C29-C30-C31-C32
25	c	612	CLA	C2-C1-O2A-CGA
25	B	607	CLA	C13-C15-C16-C17
24	Y	305	CHL	CAA-CBA-CGA-O1A
30	A	612	LHG	C29-C30-C31-C32
33	B	619	LMG	C7-C8-C9-O8
33	C	618	LMG	C7-C8-C9-O8
24	s	402	CHL	C2C-C3C-CAC-CBC
25	c	604	CLA	C10-C11-C12-C13
25	B	612	CLA	C2A-CAA-CBA-CGA
25	b	612	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	CAA-CBA-CGA-O1A
30	y	319	LHG	O10-C23-C24-C25
25	9	306	CLA	C5-C6-C7-C8
30	4	318	LHG	C25-C26-C27-C28
30	y	319	LHG	C9-C10-C11-C12
24	Y	312	CHL	C4-C3-C5-C6
25	Y	316	CLA	C4-C3-C5-C6
24	r	308	CHL	CAA-CBA-CGA-O2A
25	C	605	CLA	CAA-CBA-CGA-O2A
25	c	605	CLA	CAA-CBA-CGA-O2A
30	Y	318	LHG	O10-C23-C24-C25
30	D	407	LHG	O9-C7-C8-C9
25	r	311	CLA	CAA-CBA-CGA-O1A
24	2	306	CHL	C4B-C3B-CAB-CBB
24	3	308	CHL	C4B-C3B-CAB-CBB
24	S	605	CHL	C4B-C3B-CAB-CBB
24	S	613	CHL	C4B-C3B-CAB-CBB
24	N	305	CHL	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Y	317	CHL	C4B-C3B-CAB-CBB
24	5	310	CHL	C4B-C3B-CAB-CBB
24	y	311	CHL	C4B-C3B-CAB-CBB
24	y	318	CHL	C4B-C3B-CAB-CBB
24	p	309	CHL	C4B-C3B-CAB-CBB
24	s	406	CHL	C4B-C3B-CAB-CBB
24	s	414	CHL	C4B-C3B-CAB-CBB
24	r	303	CHL	C4B-C3B-CAB-CBB
25	R	613	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
25	b	615	CLA	C4B-C3B-CAB-CBB
25	r	314	CLA	C4B-C3B-CAB-CBB
30	2	319	LHG	C4-O6-P-O5
30	Y	318	LHG	C4-O6-P-O5
30	4	318	LHG	C4-O6-P-O5
30	5	319	LHG	C4-O6-P-O5
30	n	318	LHG	C4-O6-P-O4
30	y	319	LHG	C4-O6-P-O5
30	D	408	LHG	C7-C8-C9-C10
24	y	306	CHL	CAA-CBA-CGA-O1A
30	D	408	LHG	O6-C4-C5-C6
33	w	201	LMG	C12-C13-C14-C15
24	4	305	CHL	CAA-CBA-CGA-O1A
31	b	617	8CT	C02-C03-C10-C11
25	B	602	CLA	C5-C6-C7-C8
25	c	607	CLA	C15-C16-C17-C18
25	B	606	CLA	CAA-CBA-CGA-O1A
30	d	407	LHG	O9-C7-C8-C9
25	G	317	CLA	O1A-CGA-O2A-C1
24	s	406	CHL	CAA-CBA-CGA-O1A
25	a	604	CLA	C2A-CAA-CBA-CGA
24	Y	304	CHL	C13-C15-C16-C17
30	y	319	LHG	C31-C32-C33-C34
24	S	605	CHL	CAA-CBA-CGA-O1A
25	n	306	CLA	CAA-CBA-CGA-O2A
30	Y	318	LHG	C31-C32-C33-C34
25	C	601	CLA	CAA-CBA-CGA-O1A
30	a	601	LHG	C14-C15-C16-C17
24	q	309	CHL	C3-C5-C6-C7
24	S	601	CHL	CAD-CBD-CGD-O1D
24	S	602	CHL	CAD-CBD-CGD-O1D
24	G	305	CHL	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	9	305	CHL	CAD-CBD-CGD-O1D
24	6	305	CHL	CAD-CBD-CGD-O1D
24	g	305	CHL	CAD-CBD-CGD-O1D
24	7	313	CHL	CAD-CBD-CGD-O1D
25	R	612	CLA	CAD-CBD-CGD-O1D
25	9	314	CLA	CAD-CBD-CGD-O1D
25	N	316	CLA	CAD-CBD-CGD-O1D
25	Y	316	CLA	CAD-CBD-CGD-O1D
25	B	604	CLA	CAD-CBD-CGD-O1D
25	y	317	CLA	CAD-CBD-CGD-O1D
25	b	604	CLA	CAD-CBD-CGD-O1D
25	r	313	CLA	CAD-CBD-CGD-O1D
32	B	618	SQD	C5-C6-S-O9
32	b	618	SQD	C5-C6-S-O9
24	R	607	CHL	CAA-CBA-CGA-O2A
33	B	619	LMG	O8-C28-C29-C30
24	9	304	CHL	C6-C7-C8-C9
24	g	305	CHL	C11-C12-C13-C14
24	s	403	CHL	C11-C10-C8-C9
25	Y	314	CLA	C11-C10-C8-C9
25	C	603	CLA	C14-C13-C15-C16
25	C	611	CLA	C11-C12-C13-C14
25	p	307	CLA	C6-C7-C8-C9
25	c	603	CLA	C14-C13-C15-C16
25	c	611	CLA	C11-C12-C13-C14
24	q	308	CHL	O1D-CGD-O2D-CED
24	4	308	CHL	CBD-CGD-O2D-CED
25	B	614	CLA	CAA-CBA-CGA-O1A
25	c	601	CLA	CAA-CBA-CGA-O1A
24	3	305	CHL	CAA-CBA-CGA-O2A
24	6	309	CHL	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
25	B	612	CLA	O1A-CGA-O2A-C1
25	r	310	CLA	O1A-CGA-O2A-C1
30	2	319	LHG	C25-C26-C27-C28
25	b	607	CLA	C13-C15-C16-C17
24	g	310	CHL	C2A-CAA-CBA-CGA
24	u	313	CHL	C2C-C3C-CAC-CBC
24	3	309	CHL	CAA-CBA-CGA-O2A
24	S	602	CHL	CAA-CBA-CGA-O2A
24	G	310	CHL	CAA-CBA-CGA-O2A
24	g	306	CHL	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	7	306	CHL	CAA-CBA-CGA-O2A
25	9	307	CLA	CAA-CBA-CGA-O2A
37	c	619	DGD	O2G-C1B-C2B-C3B
24	s	407	CHL	CAA-CBA-CGA-O2A
37	c	618	DGD	C5A-C6A-C7A-C8A
30	d	407	LHG	C9-C10-C11-C12
25	y	317	CLA	C4-C3-C5-C6
25	C	607	CLA	C15-C16-C17-C18
30	n	318	LHG	C11-C12-C13-C14
24	G	306	CHL	C6-C7-C8-C10
24	Y	304	CHL	C6-C7-C8-C10
24	g	313	CHL	C11-C12-C13-C15
24	u	306	CHL	C11-C12-C13-C15
24	y	306	CHL	C6-C7-C8-C10
25	2	315	CLA	C11-C10-C8-C7
25	Y	314	CLA	C12-C13-C15-C16
25	B	605	CLA	C12-C13-C15-C16
25	C	611	CLA	C11-C12-C13-C15
25	C	616	CLA	C3A-C2A-CAA-CBA
25	5	315	CLA	C11-C10-C8-C7
25	n	314	CLA	C6-C7-C8-C10
25	y	315	CLA	C2-C3-C5-C6
25	b	605	CLA	C12-C13-C15-C16
25	c	604	CLA	C12-C13-C15-C16
25	c	616	CLA	C3A-C2A-CAA-CBA
25	d	404	CLA	C12-C13-C15-C16
26	1	302	0IE	O1-C2-C3-C20
26	2	302	0IE	O1-C2-C3-C20
26	3	302	0IE	O1-C2-C3-C20
26	G	302	0IE	O1-C2-C3-C20
26	9	302	0IE	O1-C2-C3-C20
26	N	302	0IE	O1-C2-C3-C20
26	Y	302	0IE	O1-C2-C3-C20
26	8	302	0IE	O1-C2-C3-C20
26	4	302	0IE	O1-C2-C3-C20
26	5	302	0IE	O1-C2-C3-C20
26	6	302	0IE	O1-C2-C3-C20
26	u	302	0IE	O1-C2-C3-C20
26	n	302	0IE	O1-C2-C3-C20
26	y	302	0IE	O1-C2-C3-C20
26	p	302	0IE	O1-C2-C3-C20
26	q	302	0IE	O1-C2-C3-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	7	302	0IE	O1-C2-C3-C20
29	1	301	0UR	O42-C2-C3-C43
29	9	301	0UR	C3-C2-C41-C1
29	Y	301	0UR	C3-C2-C41-C1
29	8	301	0UR	C3-C2-C41-C1
29	4	301	0UR	O42-C2-C3-C43
29	u	301	0UR	C3-C2-C41-C1
29	y	301	0UR	C3-C2-C41-C1
29	q	301	0UR	C3-C2-C41-C1
31	B	617	8CT	C28-C29-C30-C31
31	b	617	8CT	C28-C29-C30-C31
35	A	606	PHO	C12-C13-C15-C16
39	D	406	PL9	C28-C29-C31-C32
24	R	607	CHL	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A
32	a	609	SQD	O49-C7-C8-C9
24	S	606	CHL	CAA-CBA-CGA-O1A
24	G	312	CHL	CAA-CBA-CGA-O2A
24	6	305	CHL	CAA-CBA-CGA-O2A
24	g	312	CHL	CAA-CBA-CGA-O2A
24	p	306	CHL	CAA-CBA-CGA-O2A
24	s	403	CHL	CAA-CBA-CGA-O2A
25	N	306	CLA	CAA-CBA-CGA-O2A
25	Y	306	CLA	CAA-CBA-CGA-O2A
25	y	307	CLA	CAA-CBA-CGA-O2A
25	d	404	CLA	CAA-CBA-CGA-O2A
24	S	602	CHL	CAA-CBA-CGA-O1A
24	G	312	CHL	CAA-CBA-CGA-O1A
24	6	305	CHL	CAA-CBA-CGA-O1A
24	s	403	CHL	CAA-CBA-CGA-O1A
24	7	306	CHL	CAA-CBA-CGA-O1A
25	N	306	CLA	CAA-CBA-CGA-O1A
25	C	605	CLA	CAA-CBA-CGA-O1A
25	c	605	CLA	CAA-CBA-CGA-O1A
29	N	301	0UR	C3-C4-C5-C6
29	y	301	0UR	C3-C4-C5-C6
25	r	304	CLA	CAA-CBA-CGA-O2A
24	5	305	CHL	C4C-C3C-CAC-CBC
24	6	309	CHL	CAA-CBA-CGA-O1A
24	g	306	CHL	CAA-CBA-CGA-O1A
25	n	306	CLA	CAA-CBA-CGA-O1A
25	r	304	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	D	406	PL9	C39-C41-C42-C43
39	d	406	PL9	C34-C36-C37-C38
24	S	606	CHL	CAA-CBA-CGA-O2A
25	C	610	CLA	C8-C10-C11-C12
30	Y	318	LHG	C11-C12-C13-C14
24	G	306	CHL	CAA-CBA-CGA-O2A
25	n	313	CLA	CAA-CBA-CGA-O2A
25	p	308	CLA	CAA-CBA-CGA-O2A
24	r	308	CHL	CAA-CBA-CGA-O1A
33	B	619	LMG	O10-C28-C29-C30
25	C	602	CLA	C10-C11-C12-C13
30	a	601	LHG	C18-C19-C20-C21
24	G	310	CHL	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
24	Y	319	CHL	C3-C5-C6-C7
24	R	606	CHL	CAA-CBA-CGA-O2A
25	C	612	CLA	CAA-CBA-CGA-O2A
24	s	407	CHL	CAA-CBA-CGA-O1A

There are no ring outliers.

435 monomers are involved in 1342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	313	CHL	10	0
25	1	307	CLA	9	0
25	G	314	CLA	2	0
25	y	316	CLA	3	0
25	7	316	CLA	3	0
24	4	310	CHL	3	0
29	u	301	0UR	1	0
24	q	308	CHL	3	0
30	d	407	LHG	7	0
25	R	609	CLA	1	0
24	R	606	CHL	2	0
26	R	614	0IE	1	0
30	G	319	LHG	1	0
25	C	609	CLA	2	0
30	9	318	LHG	6	0
24	q	304	CHL	4	0
25	4	314	CLA	1	0
30	5	319	LHG	2	0
25	3	316	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	7	308	CLA	15	0
37	C	619	DGD	5	0
25	s	413	CLA	1	0
24	2	305	CHL	5	0
25	Y	306	CLA	2	0
25	3	307	CLA	2	0
24	s	408	CHL	1	0
24	G	309	CHL	2	0
25	g	317	CLA	1	0
25	u	314	CLA	2	0
25	r	305	CLA	9	0
25	y	314	CLA	2	0
30	A	612	LHG	2	0
25	9	316	CLA	4	0
24	g	306	CHL	3	0
24	u	318	CHL	1	0
24	Y	312	CHL	7	0
24	1	311	CHL	7	0
24	y	310	CHL	1	0
25	C	602	CLA	2	0
24	5	305	CHL	6	0
25	B	606	CLA	8	0
25	A	604	CLA	5	0
28	N	303	NEX	7	0
25	B	610	CLA	2	0
25	n	306	CLA	2	0
24	S	607	CHL	2	0
32	D	409	SQD	1	0
24	q	303	CHL	3	0
25	6	306	CLA	1	0
24	r	309	CHL	2	0
25	s	410	CLA	4	0
25	B	608	CLA	6	0
31	V	401	8CT	1	0
25	R	612	CLA	7	0
24	u	309	CHL	2	0
28	p	304	NEX	27	0
24	S	605	CHL	2	0
23	f	201	HEM	3	0
25	2	316	CLA	1	0
24	p	305	CHL	7	0
24	q	311	CHL	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	u	306	CHL	4	0
24	1	317	CHL	2	0
30	n	318	LHG	4	0
24	2	313	CHL	3	0
25	D	405	CLA	5	0
24	y	311	CHL	1	0
24	N	304	CHL	5	0
24	S	613	CHL	2	0
30	7	319	LHG	3	0
26	7	302	0IE	2	0
24	9	311	CHL	4	0
25	9	307	CLA	4	0
25	A	607	CLA	2	0
25	y	307	CLA	2	0
25	C	605	CLA	1	0
28	g	304	NEX	15	0
24	N	309	CHL	1	0
24	S	601	CHL	1	0
24	n	308	CHL	3	0
31	v	401	8CT	1	0
25	3	306	CLA	1	0
25	b	604	CLA	10	0
25	C	611	CLA	5	0
24	7	312	CHL	6	0
25	n	307	CLA	4	0
24	4	308	CHL	1	0
25	9	313	CLA	2	0
25	C	607	CLA	2	0
24	n	312	CHL	2	0
25	r	311	CLA	1	0
25	B	602	CLA	7	0
33	w	201	LMG	6	0
24	9	317	CHL	1	0
26	6	302	0IE	2	0
37	c	618	DGD	4	0
25	7	315	CLA	2	0
25	C	604	CLA	4	0
24	y	312	CHL	4	0
30	y	319	LHG	2	0
30	D	407	LHG	7	0
25	g	314	CLA	2	0
25	b	614	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	N	310	CHL	2	0
24	p	311	CHL	2	0
25	c	608	CLA	3	0
24	9	308	CHL	1	0
25	u	315	CLA	4	0
29	9	301	0UR	1	0
26	y	302	0IE	1	0
24	3	311	CHL	6	0
24	r	303	CHL	5	0
24	4	317	CHL	2	0
25	y	315	CLA	3	0
25	G	307	CLA	2	0
25	8	311	CLA	2	0
24	y	305	CHL	8	0
24	7	305	CHL	6	0
25	G	317	CLA	2	0
24	r	308	CHL	3	0
25	b	605	CLA	4	0
29	6	301	0UR	1	0
26	3	302	0IE	2	0
25	C	612	CLA	2	0
24	g	311	CHL	3	0
28	s	401	NEX	21	0
24	N	311	CHL	4	0
25	1	316	CLA	2	0
28	u	304	NEX	9	0
25	5	315	CLA	1	0
24	Y	305	CHL	2	0
26	u	302	0IE	1	0
32	b	618	SQD	5	0
24	8	309	CHL	5	0
25	s	412	CLA	3	0
25	b	610	CLA	3	0
25	b	609	CLA	4	0
25	c	604	CLA	3	0
25	a	607	CLA	2	0
30	a	612	LHG	2	0
24	6	311	CHL	9	0
25	5	314	CLA	2	0
25	b	612	CLA	8	0
29	2	301	0UR	1	0
24	S	602	CHL	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	N	308	CHL	3	0
24	G	318	CHL	1	0
25	u	316	CLA	4	0
25	a	604	CLA	6	0
25	1	314	CLA	1	0
25	N	316	CLA	4	0
26	9	302	0IE	2	0
25	Y	315	CLA	1	0
24	3	305	CHL	1	0
25	r	313	CLA	5	0
25	c	611	CLA	3	0
24	Y	311	CHL	4	0
28	R	616	NEX	6	0
25	1	313	CLA	2	0
24	9	312	CHL	3	0
25	5	308	CLA	5	0
25	c	612	CLA	4	0
24	1	305	CHL	2	0
24	G	306	CHL	6	0
25	q	314	CLA	1	0
25	G	316	CLA	3	0
24	6	309	CHL	20	0
24	s	402	CHL	3	0
24	2	312	CHL	2	0
33	d	401	LMG	3	0
25	B	612	CLA	8	0
24	4	309	CHL	7	0
24	R	608	CHL	2	0
24	6	310	CHL	2	0
25	R	604	CLA	7	0
25	n	316	CLA	4	0
25	c	605	CLA	2	0
25	4	316	CLA	2	0
25	s	417	CLA	4	0
27	r	316	XAT	8	0
24	5	312	CHL	3	0
33	D	411	LMG	5	0
24	y	318	CHL	2	0
25	8	312	CLA	1	0
26	Y	302	0IE	1	0
24	g	312	CHL	3	0
24	q	307	CHL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	615	CLA	8	0
25	R	610	CLA	1	0
25	5	317	CLA	2	0
24	7	313	CHL	3	0
25	b	607	CLA	3	0
31	C	613	8CT	1	0
25	p	308	CLA	12	0
24	4	304	CHL	2	0
24	q	310	CHL	6	0
24	s	403	CHL	3	0
25	p	317	CLA	5	0
24	3	309	CHL	19	0
25	7	317	CLA	4	0
25	C	601	CLA	4	0
24	r	306	CHL	3	0
24	u	312	CHL	4	0
24	8	310	CHL	6	0
25	c	616	CLA	2	0
29	Y	301	0UR	1	0
25	4	315	CLA	2	0
25	c	607	CLA	3	0
25	p	314	CLA	2	0
25	A	603	CLA	5	0
24	6	304	CHL	3	0
24	9	309	CHL	3	0
25	b	616	CLA	3	0
24	8	303	CHL	3	0
24	g	305	CHL	4	0
25	p	307	CLA	2	0
33	C	618	LMG	6	0
25	S	611	CLA	1	0
26	9	303	0IE	1	0
37	c	619	DGD	4	0
25	q	313	CLA	1	0
23	E	201	HEM	2	0
24	6	308	CHL	1	0
25	B	603	CLA	3	0
25	6	315	CLA	1	0
25	9	306	CLA	1	0
25	S	616	CLA	4	0
25	2	314	CLA	1	0
25	p	316	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	310	CHL	6	0
24	R	605	CHL	3	0
25	n	315	CLA	2	0
24	g	318	CHL	2	0
25	g	307	CLA	2	0
24	p	309	CHL	3	0
24	N	305	CHL	2	0
25	A	605	CLA	1	0
35	d	403	PHO	6	0
25	p	315	CLA	2	0
25	B	607	CLA	4	0
35	A	606	PHO	4	0
25	b	615	CLA	7	0
25	y	308	CLA	1	0
30	A	601	LHG	6	0
25	Y	314	CLA	1	0
25	G	308	CLA	16	0
24	n	309	CHL	1	0
25	2	317	CLA	2	0
25	B	614	CLA	3	0
26	2	303	0IE	1	0
31	c	613	8CT	1	0
25	g	316	CLA	2	0
25	3	315	CLA	1	0
25	d	404	CLA	4	0
28	r	317	NEX	9	0
24	6	317	CHL	2	0
24	G	311	CHL	4	0
25	B	616	CLA	3	0
24	1	309	CHL	5	0
25	7	314	CLA	2	0
30	D	408	LHG	6	0
24	7	306	CHL	4	0
25	q	306	CLA	5	0
25	2	308	CLA	5	0
25	D	404	CLA	5	0
25	N	315	CLA	3	0
28	2	304	NEX	9	0
28	r	301	NEX	6	0
33	W	201	LMG	2	0
24	8	307	CHL	1	0
25	7	307	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	s	409	CHL	2	0
25	y	317	CLA	2	0
29	y	301	0UR	1	0
26	y	303	0IE	1	0
25	R	603	CLA	1	0
29	G	301	0UR	1	0
25	c	603	CLA	3	0
25	d	405	CLA	6	0
29	n	301	0UR	1	0
25	q	315	CLA	1	0
24	3	317	CHL	2	0
25	S	612	CLA	1	0
25	8	313	CLA	1	0
25	4	313	CLA	2	0
24	u	305	CHL	5	0
24	p	306	CHL	4	0
29	4	301	0UR	1	0
24	5	309	CHL	1	0
25	b	601	CLA	1	0
24	Y	317	CHL	2	0
24	g	313	CHL	6	0
27	R	615	XAT	16	0
25	C	610	CLA	4	0
33	D	401	LMG	3	0
24	y	313	CHL	6	0
24	G	312	CHL	12	0
25	q	305	CLA	2	0
24	4	312	CHL	3	0
24	N	312	CHL	4	0
25	8	306	CLA	4	0
24	R	602	CHL	4	0
24	Y	309	CHL	2	0
24	u	310	CHL	4	0
24	u	311	CHL	1	0
24	S	608	CHL	1	0
25	B	609	CLA	3	0
28	5	304	NEX	10	0
25	b	611	CLA	3	0
24	p	310	CHL	12	0
25	c	601	CLA	3	0
24	u	313	CHL	1	0
24	y	309	CHL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	d	406	PL9	2	0
24	5	313	CHL	4	0
33	i	101	LMG	3	0
25	9	315	CLA	4	0
25	C	603	CLA	5	0
28	7	304	NEX	32	0
24	n	310	CHL	2	0
25	b	602	CLA	8	0
25	r	314	CLA	1	0
24	Y	304	CHL	5	0
25	5	316	CLA	2	0
24	1	310	CHL	3	0
30	g	319	LHG	2	0
29	q	301	0UR	1	0
32	d	409	SQD	1	0
25	9	314	CLA	3	0
24	8	304	CHL	6	0
37	C	620	DGD	2	0
30	a	601	LHG	5	0
24	y	306	CHL	2	0
25	B	613	CLA	5	0
25	u	307	CLA	2	0
24	n	311	CHL	4	0
24	r	307	CHL	4	0
25	g	308	CLA	6	0
24	Y	308	CHL	3	0
24	n	304	CHL	4	0
24	7	311	CHL	2	0
24	G	310	CHL	3	0
24	s	407	CHL	2	0
25	B	601	CLA	1	0
30	N	318	LHG	4	0
28	9	319	NEX	6	0
25	C	616	CLA	2	0
24	R	607	CHL	3	0
24	2	309	CHL	1	0
24	G	305	CHL	4	0
26	p	302	0IE	2	0
24	1	304	CHL	3	0
25	2	315	CLA	1	0
25	c	609	CLA	3	0
24	s	414	CHL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	312	CHL	4	0
25	B	611	CLA	5	0
24	4	305	CHL	1	0
28	1	303	NEX	22	0
24	3	308	CHL	2	0
24	7	310	CHL	14	0
25	8	305	CLA	2	0
25	b	608	CLA	5	0
30	p	319	LHG	3	0
25	u	308	CLA	1	0
25	N	307	CLA	4	0
25	a	603	CLA	5	0
32	A	609	SQD	2	0
35	D	403	PHO	6	0
24	r	302	CHL	3	0
24	p	318	CHL	3	0
25	1	315	CLA	2	0
29	8	301	0UR	1	0
24	3	304	CHL	1	0
24	5	311	CHL	1	0
24	R	601	CHL	3	0
25	b	613	CLA	5	0
24	g	309	CHL	2	0
25	r	310	CLA	1	0
25	c	602	CLA	2	0
25	g	315	CLA	3	0
30	4	318	LHG	3	0
24	Y	310	CHL	1	0
28	y	304	NEX	4	0
33	B	619	LMG	5	0
24	s	406	CHL	2	0
25	B	605	CLA	6	0
28	3	318	NEX	22	0
28	G	304	NEX	32	0
24	n	305	CHL	5	0
29	p	301	0UR	1	0
25	S	609	CLA	4	0
24	S	606	CHL	2	0
24	6	305	CHL	1	0
25	N	306	CLA	1	0
28	S	617	NEX	24	0
25	a	605	CLA	1	0

Continued on next page...

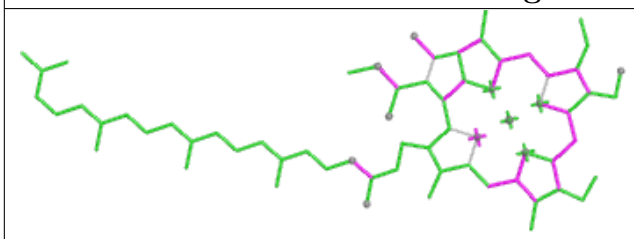
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	9	304	CHL	6	0
24	4	311	CHL	5	0
25	s	411	CLA	3	0
26	r	315	0IE	1	0
35	a	606	PHO	4	0
25	b	606	CLA	9	0
25	b	603	CLA	4	0
25	c	610	CLA	4	0
32	B	618	SQD	4	0
25	4	307	CLA	16	0
25	u	317	CLA	5	0
24	3	310	CHL	1	0
24	p	312	CHL	5	0
24	7	318	CHL	2	0
39	D	406	PL9	2	0
28	6	303	NEX	21	0
30	1	318	LHG	3	0
33	m	101	LMG	6	0
24	9	305	CHL	6	0
30	d	408	LHG	4	0
24	9	310	CHL	2	0
25	B	604	CLA	12	0
25	6	316	CLA	3	0
25	r	304	CLA	1	0
25	6	307	CLA	2	0
25	Y	316	CLA	2	0
24	8	308	CHL	3	0
25	q	312	CLA	2	0
32	a	609	SQD	4	0
24	p	313	CHL	3	0
28	n	303	NEX	7	0
25	G	315	CLA	3	0
25	Y	313	CLA	2	0
33	d	411	LMG	5	0
25	N	313	CLA	1	0
25	8	314	CLA	2	0
28	4	303	NEX	21	0
30	2	319	LHG	2	0

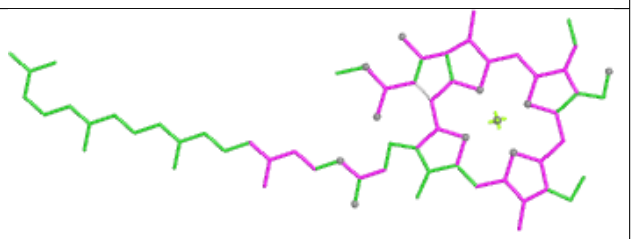
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

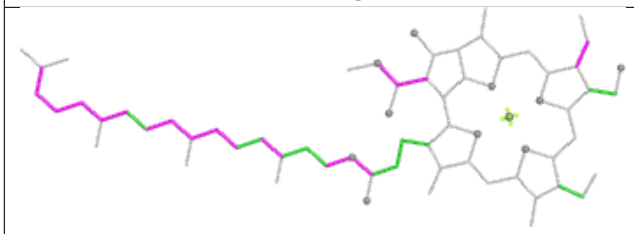
Ligand CHL G 313



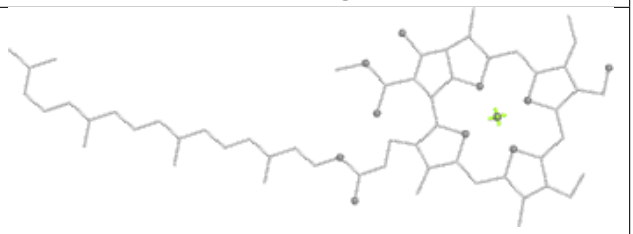
Bond lengths



Bond angles

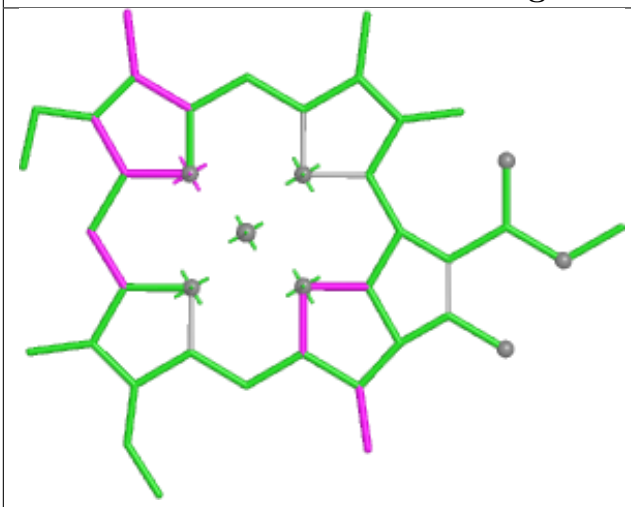


Torsions

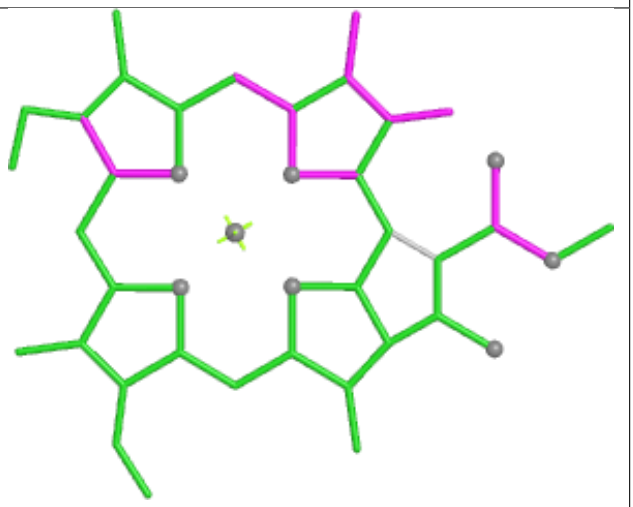


Rings

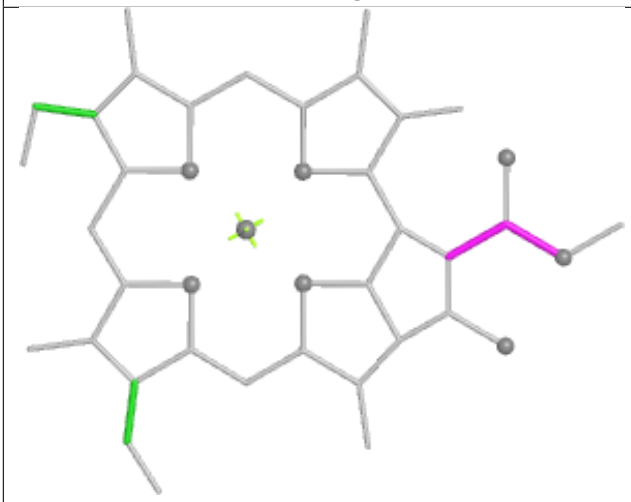
Ligand CLA 1 307



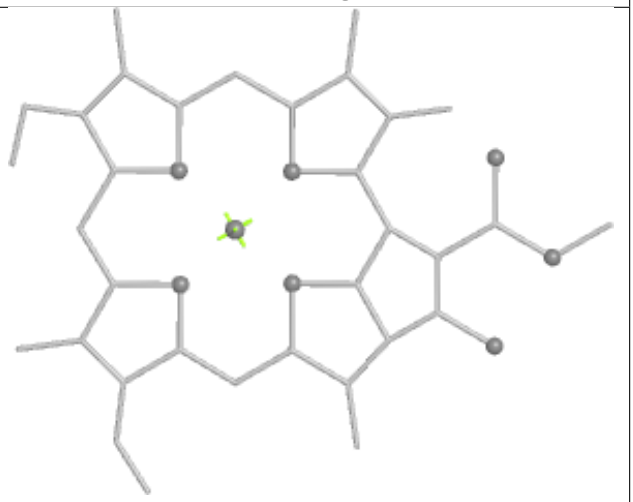
Bond lengths



Bond angles

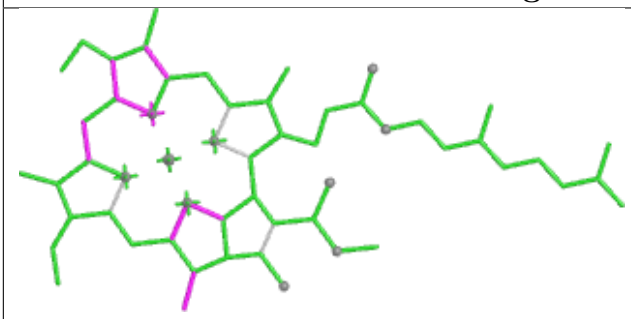


Torsions

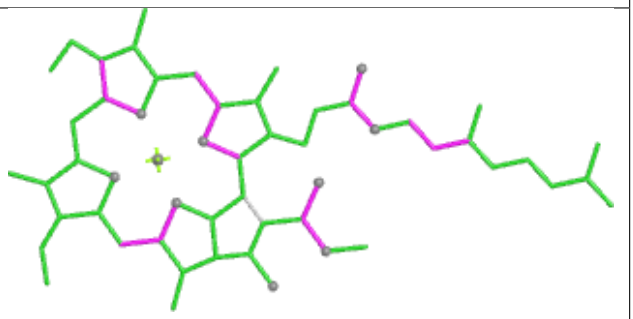


Rings

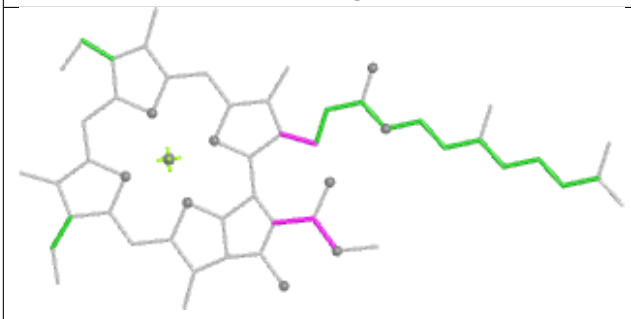
Ligand CLA G 314



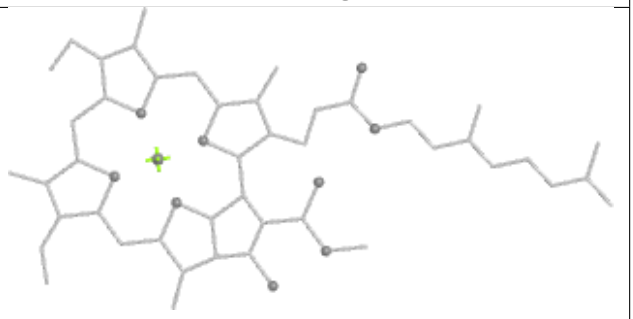
Bond lengths



Bond angles

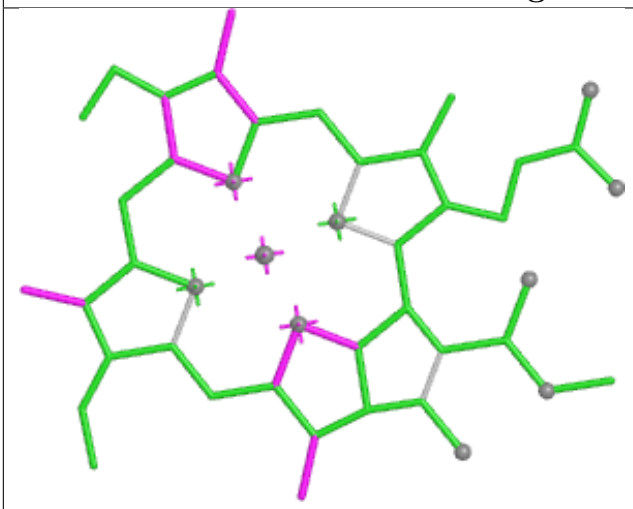


Torsions

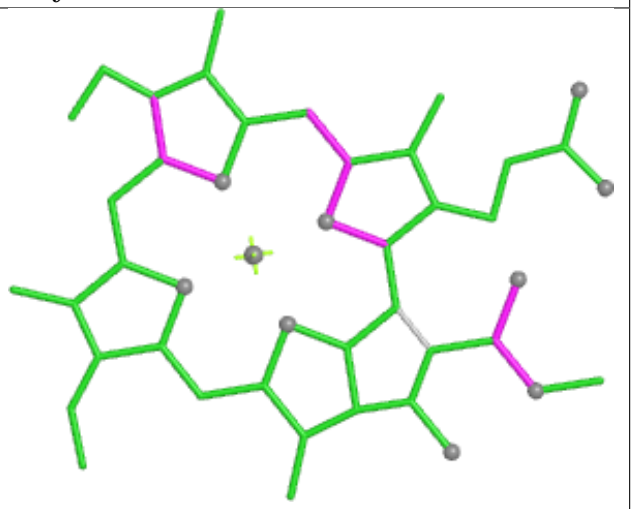


Rings

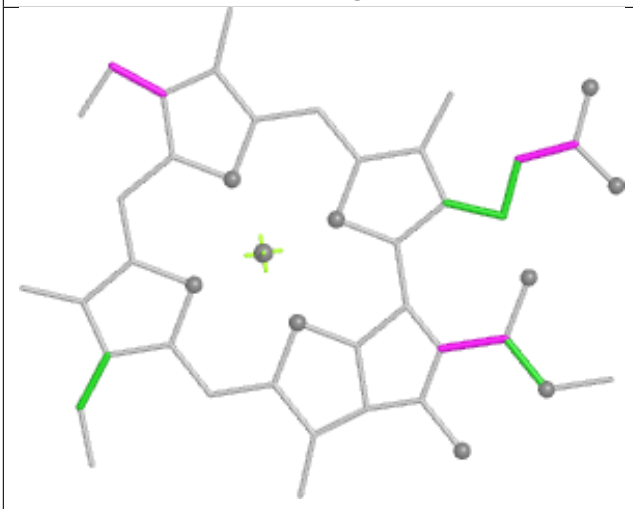
Ligand CLA y 316



Bond lengths



Bond angles

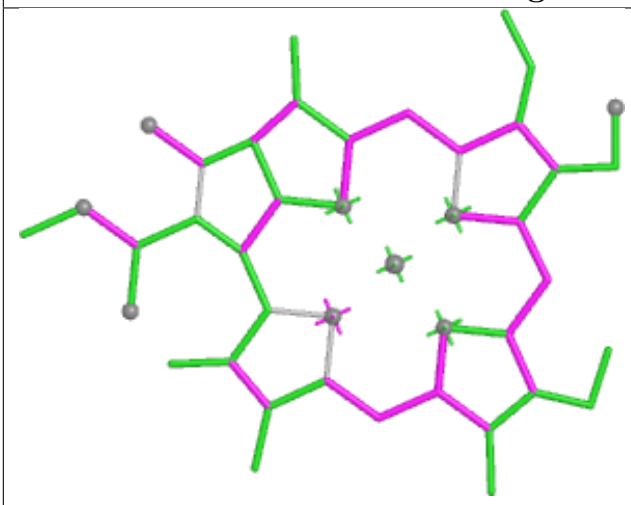


Torsions

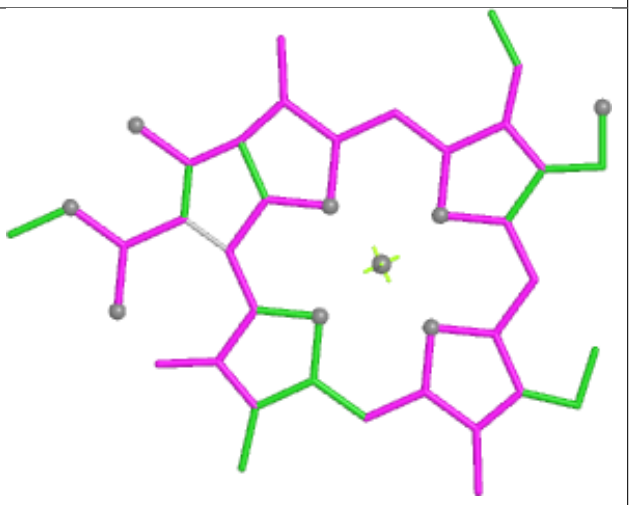


Rings

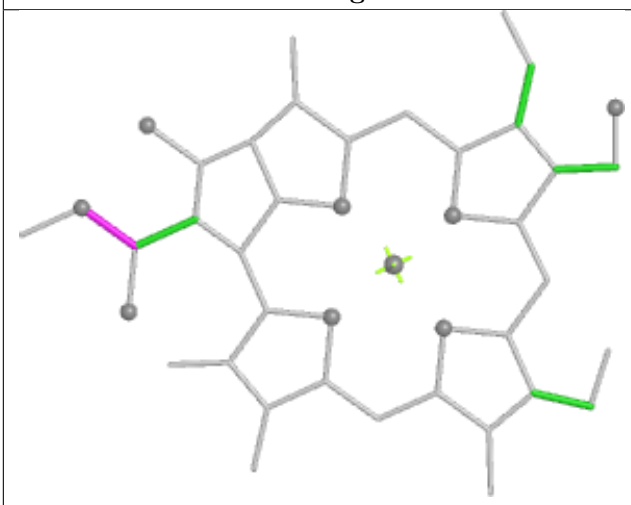
Ligand CHL 2 310



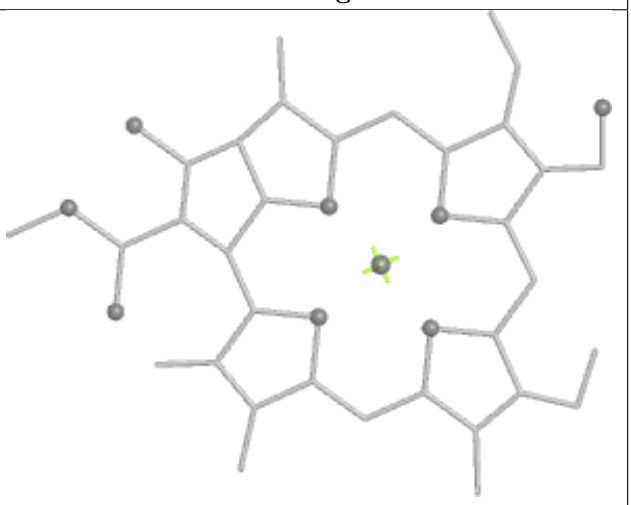
Bond lengths



Bond angles

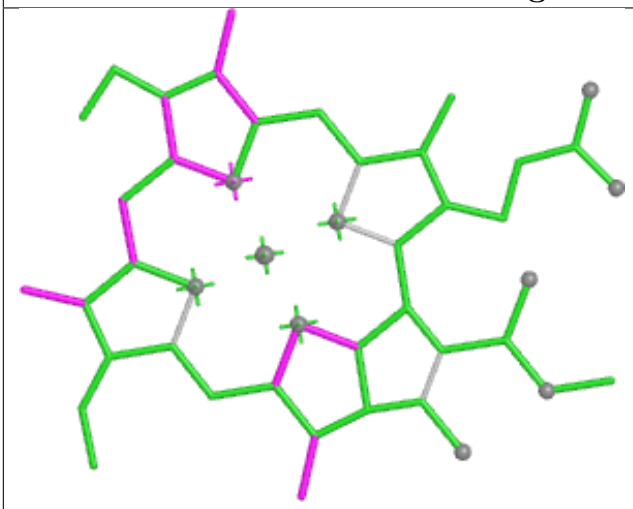


Torsions

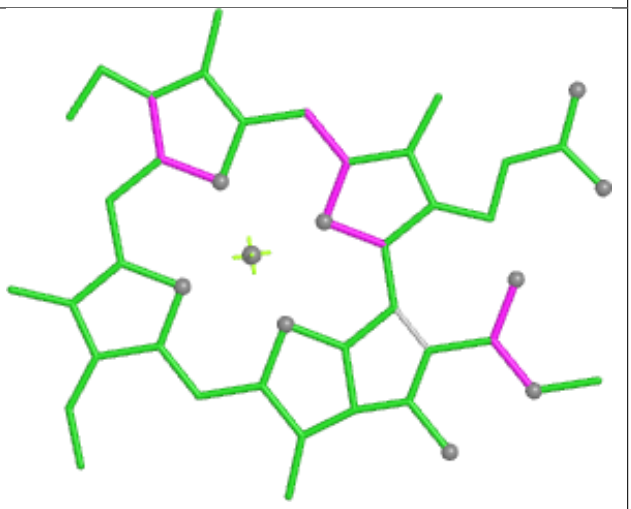


Rings

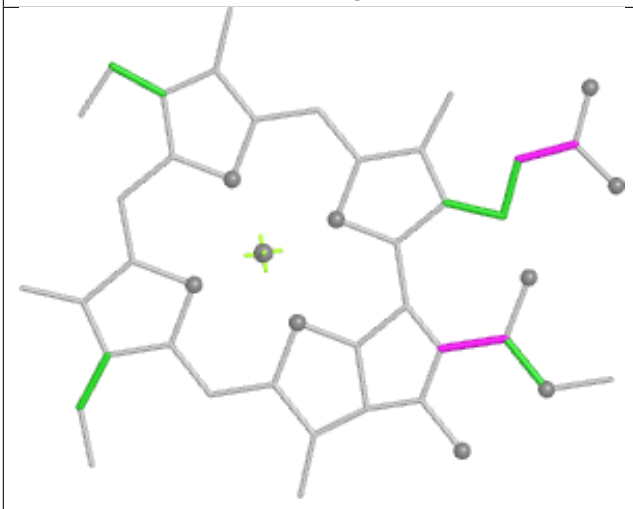
Ligand CLA 7 316



Bond lengths



Bond angles

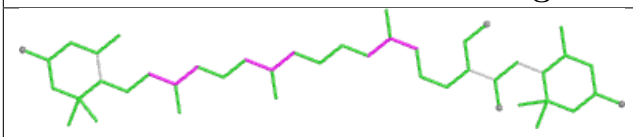


Torsions

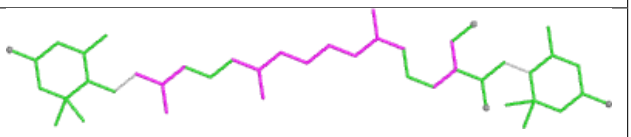


Rings

Ligand 0IE G 303



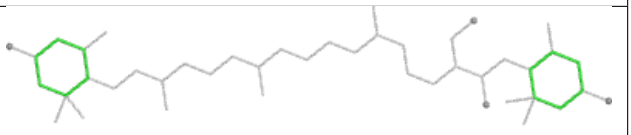
Bond lengths



Bond angles

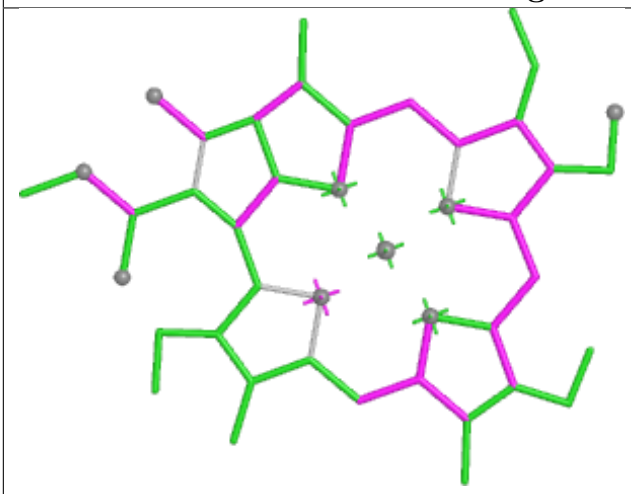


Torsions

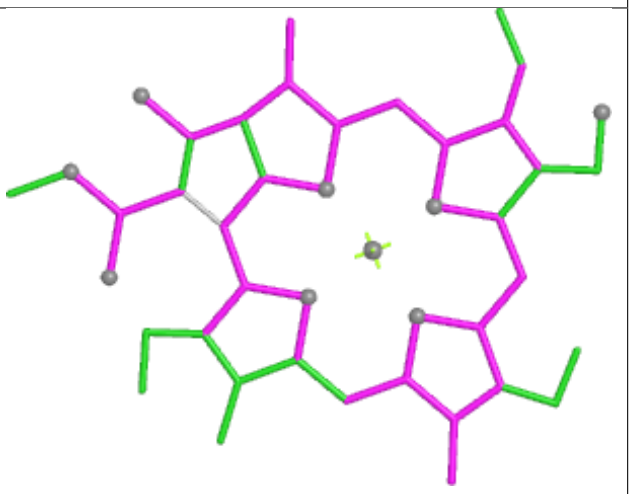


Rings

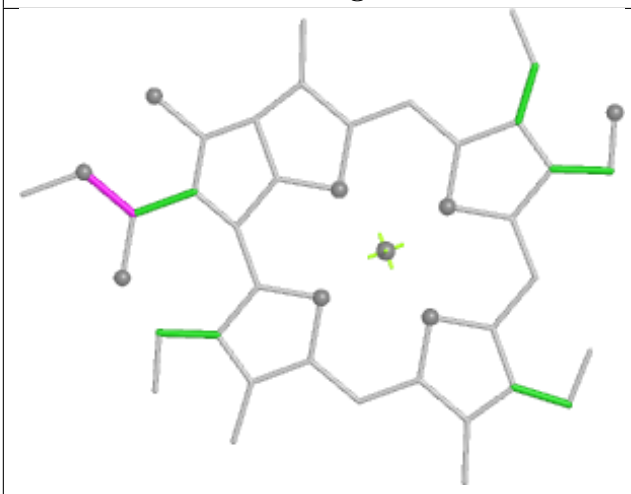
Ligand CHL 4 310



Bond lengths



Bond angles

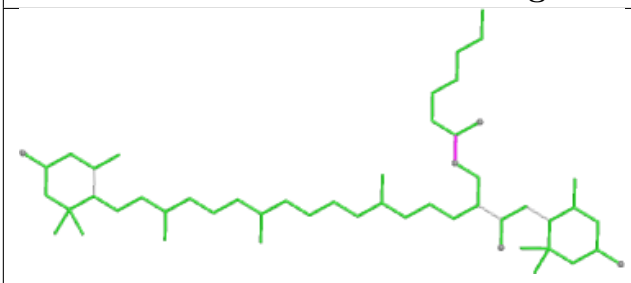


Torsions

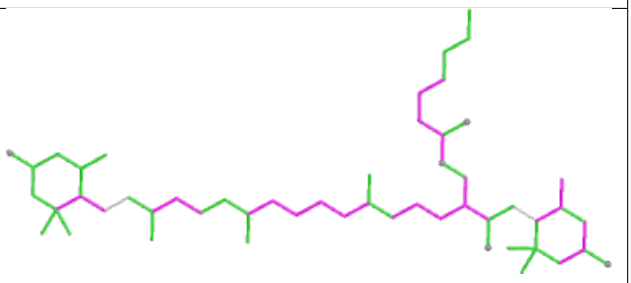


Rings

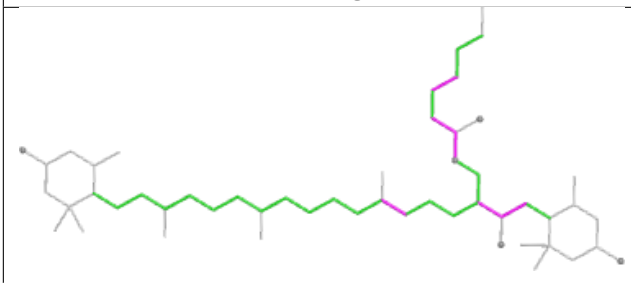
Ligand 0UR u 301



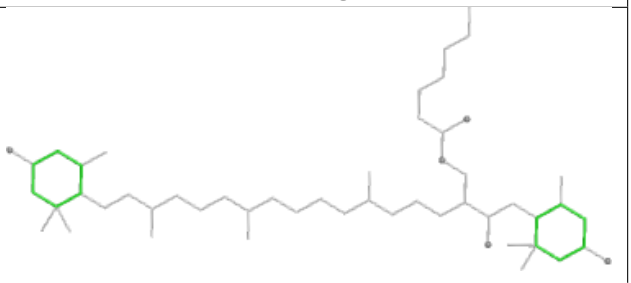
Bond lengths



Bond angles

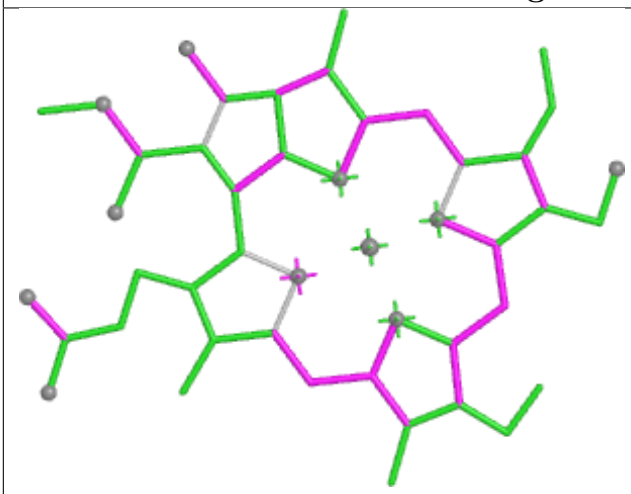


Torsions

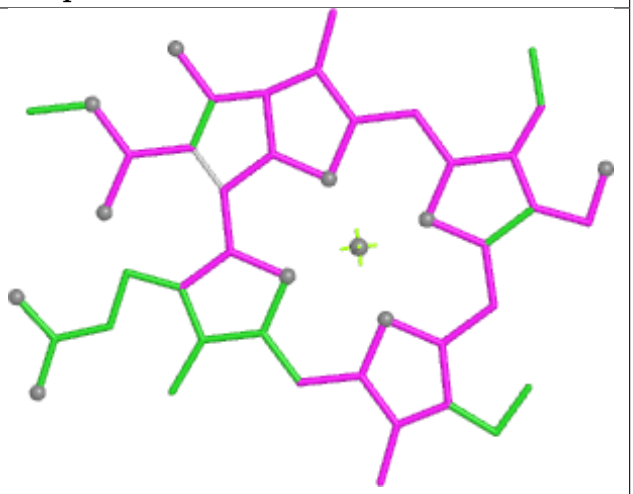


Rings

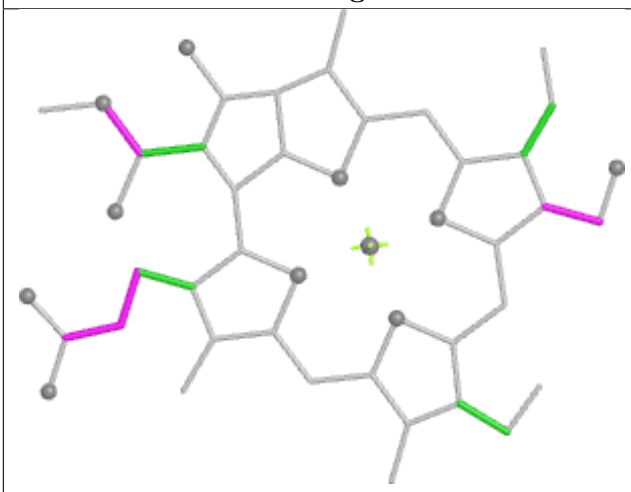
Ligand CHL q 308



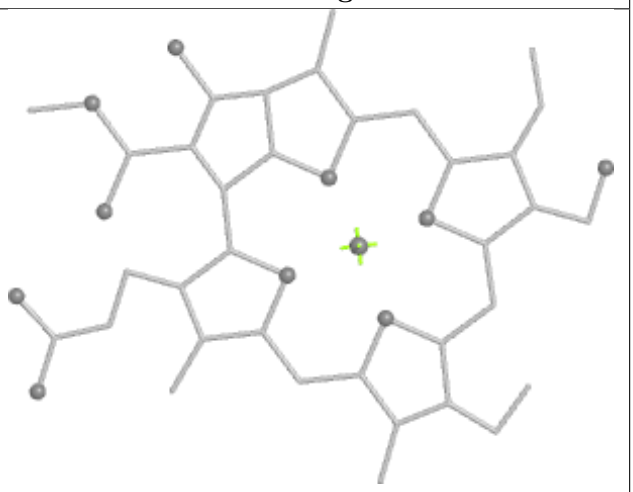
Bond lengths



Bond angles

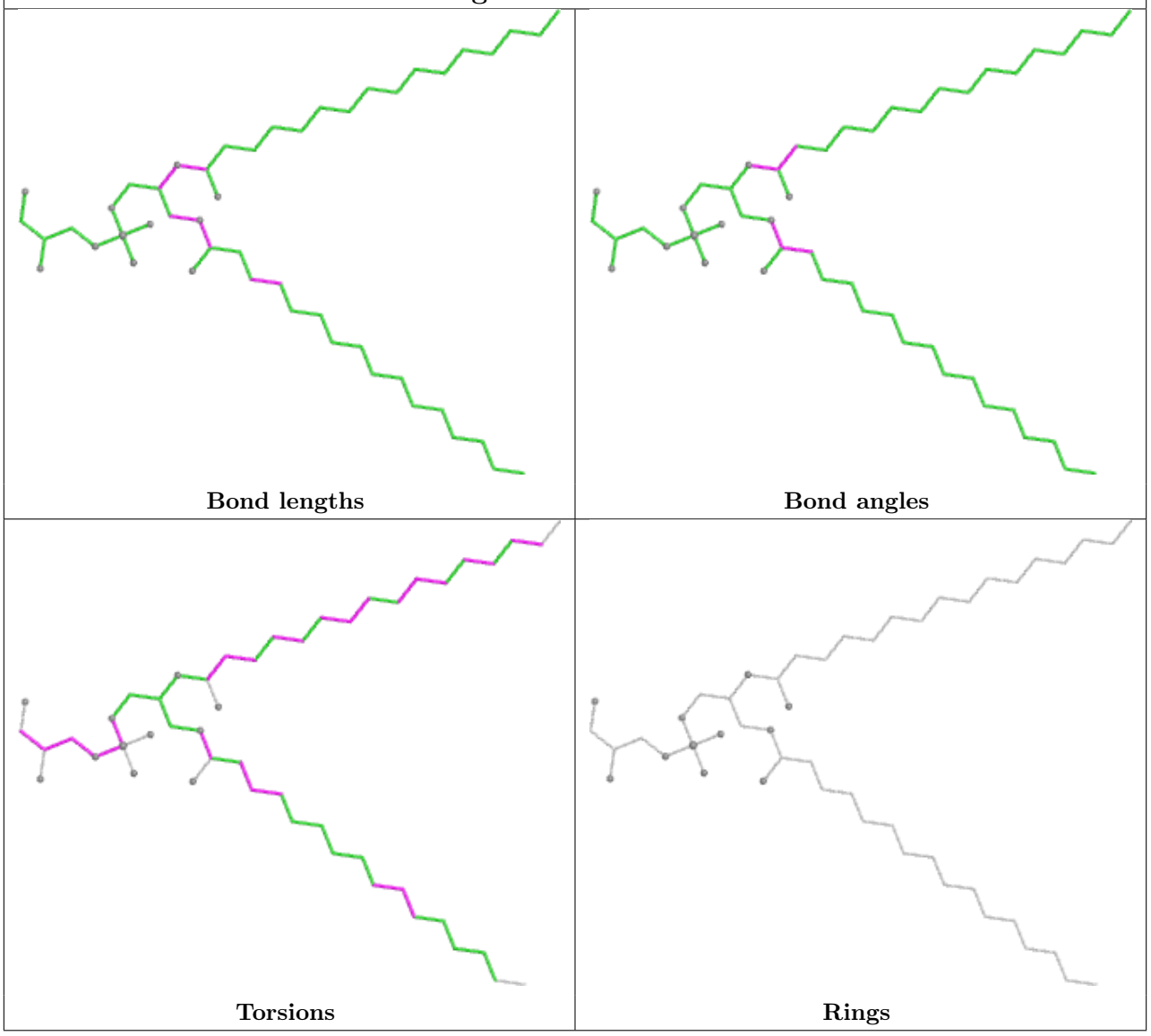


Torsions

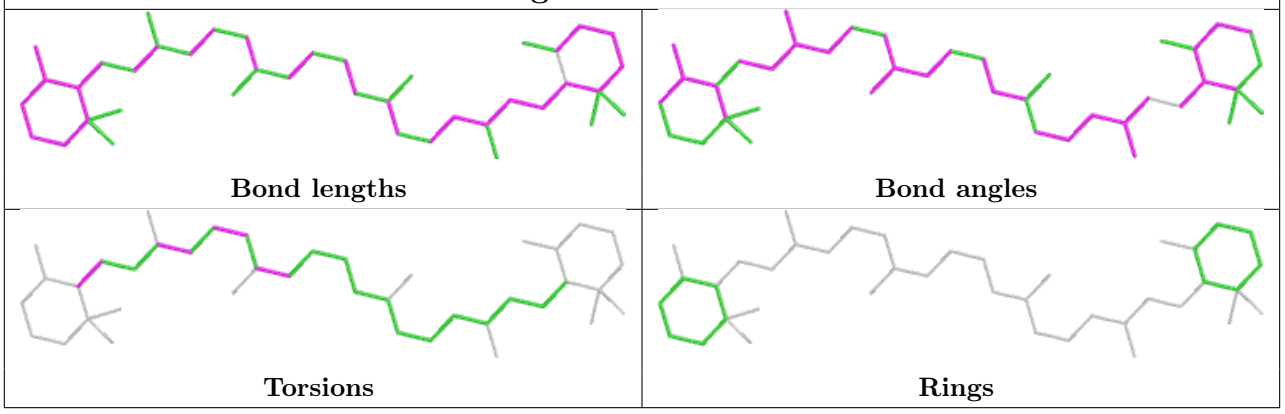


Rings

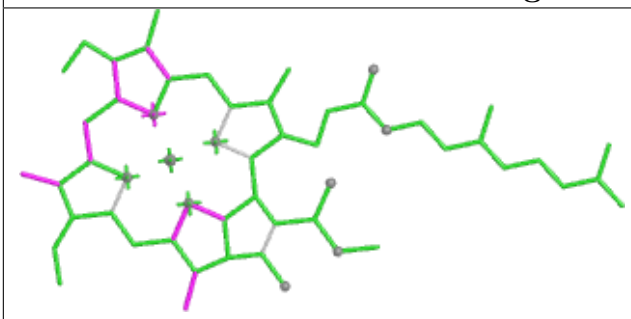
Ligand LHG d 407



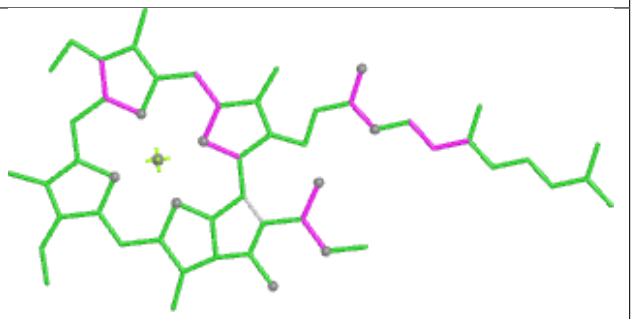
Ligand 8CT S 614



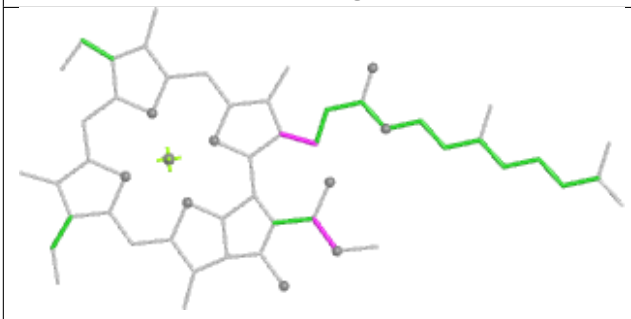
Ligand CLA R 609



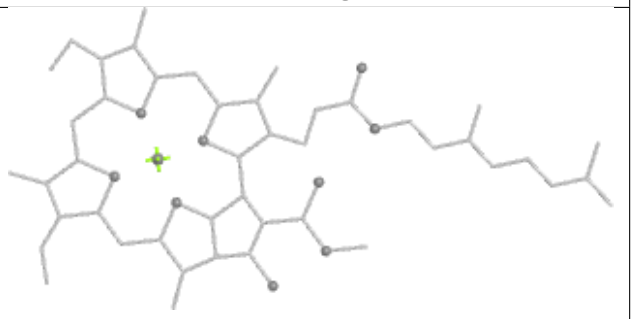
Bond lengths



Bond angles

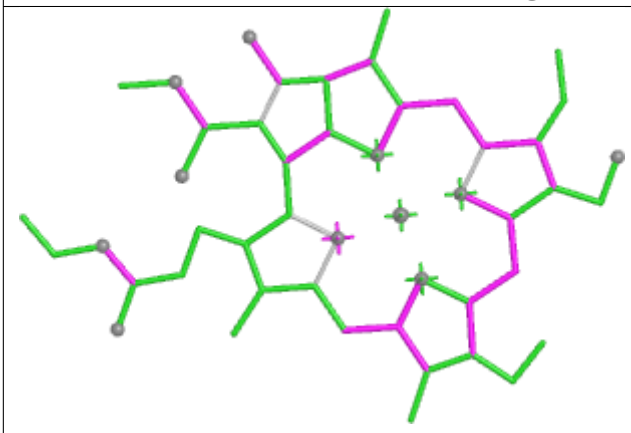


Torsions

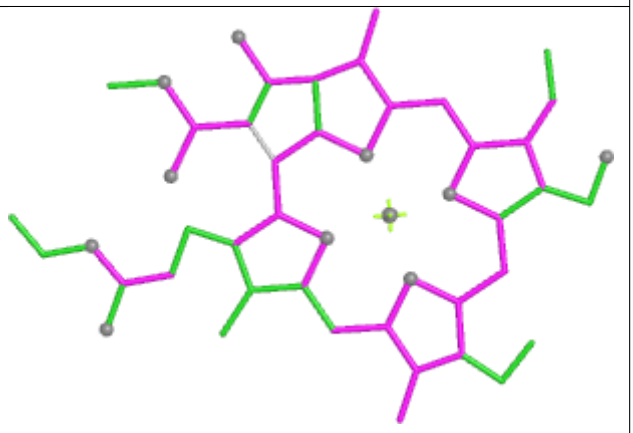


Rings

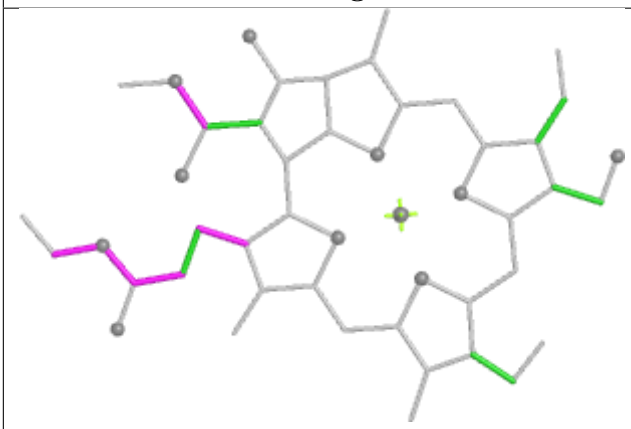
Ligand CHL R 606



Bond lengths



Bond angles

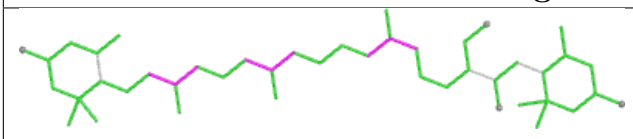


Torsions

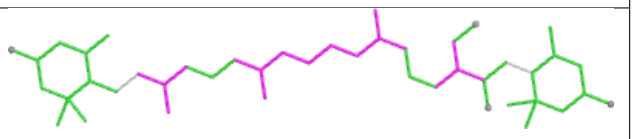


Rings

Ligand 0IE R 614



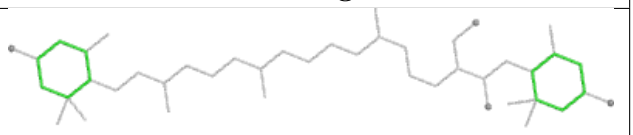
Bond lengths



Bond angles

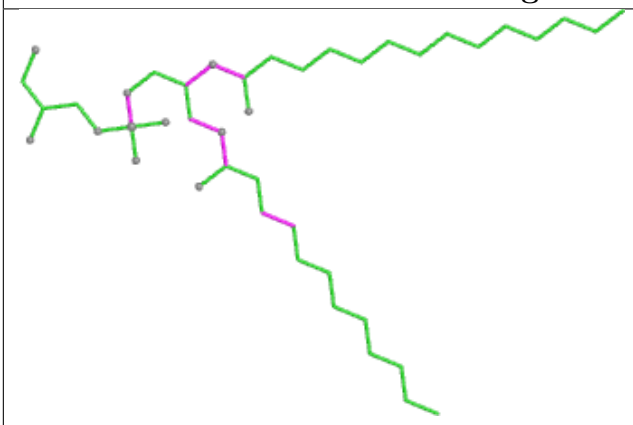


Torsions

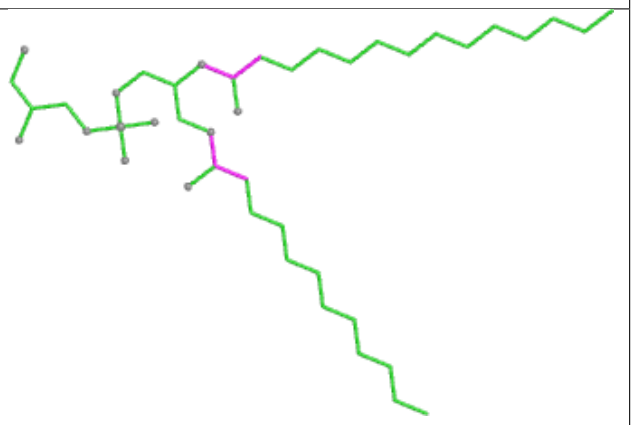


Rings

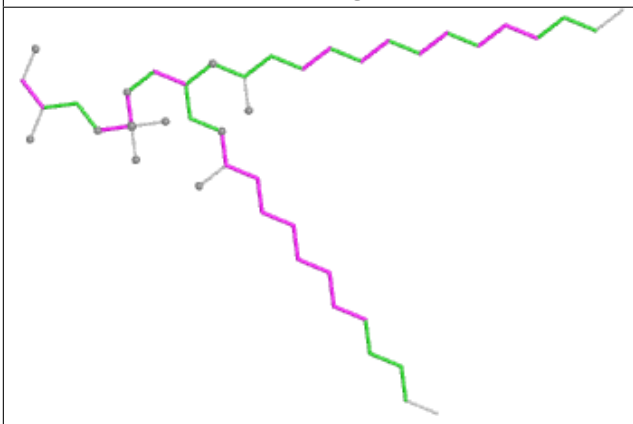
Ligand LHG G 319



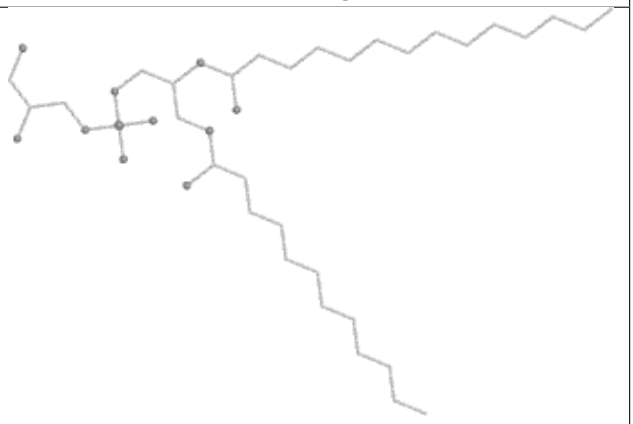
Bond lengths



Bond angles

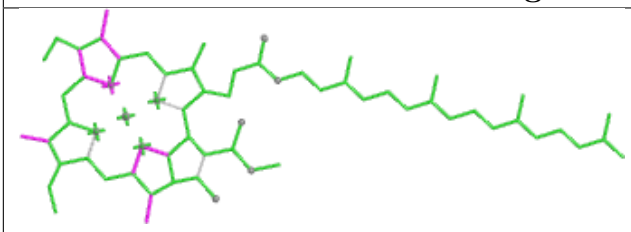


Torsions

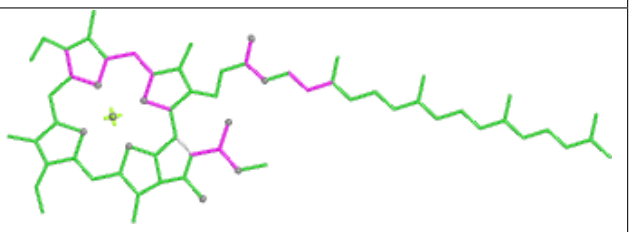


Rings

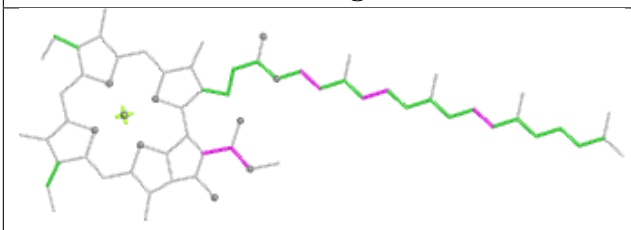
Ligand CLA C 609



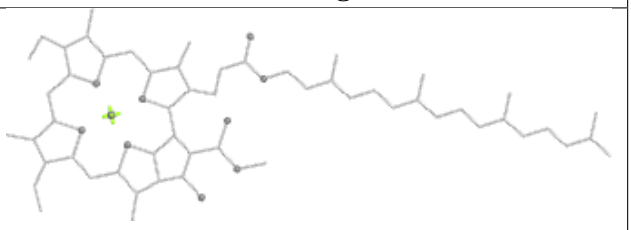
Bond lengths



Bond angles

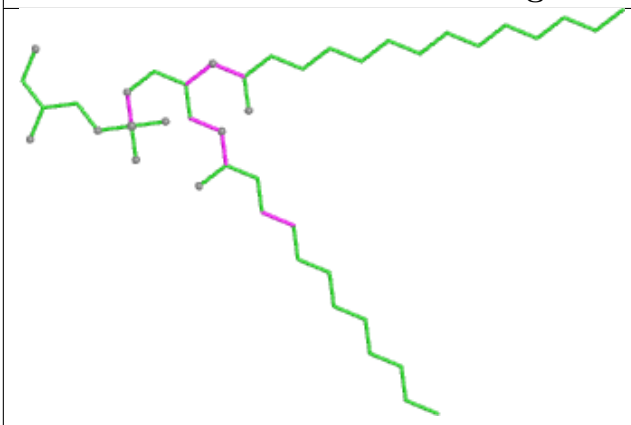


Torsions

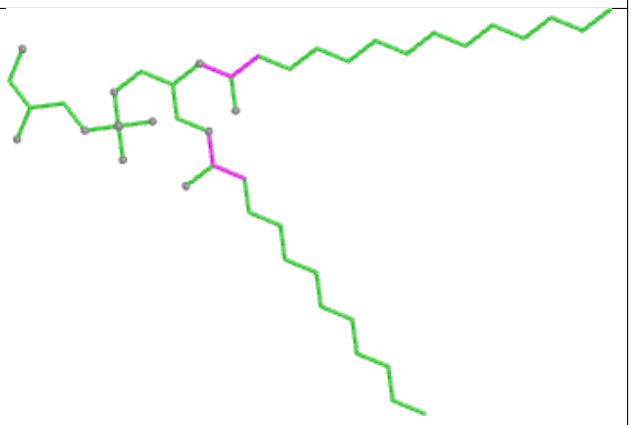


Rings

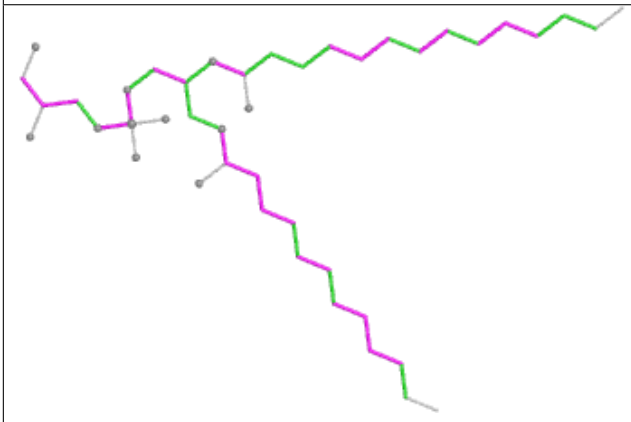
Ligand LHG 9 318



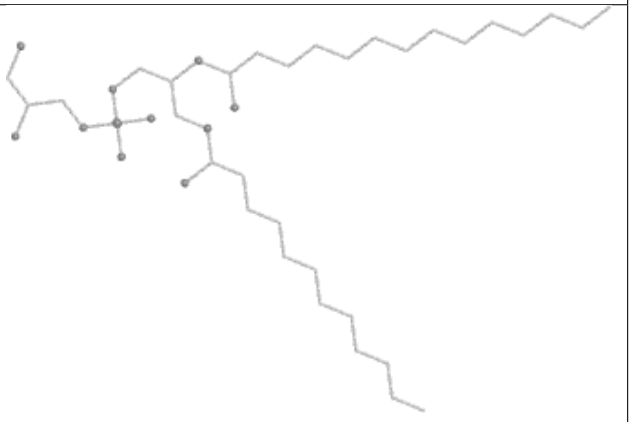
Bond lengths



Bond angles

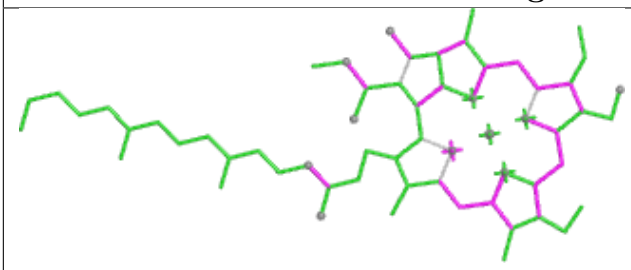


Torsions

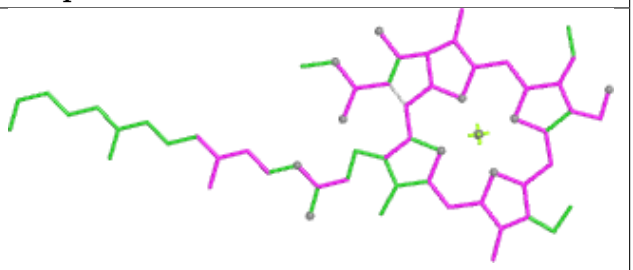


Rings

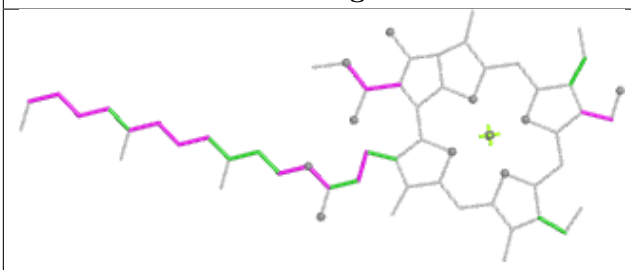
Ligand CHL q 304



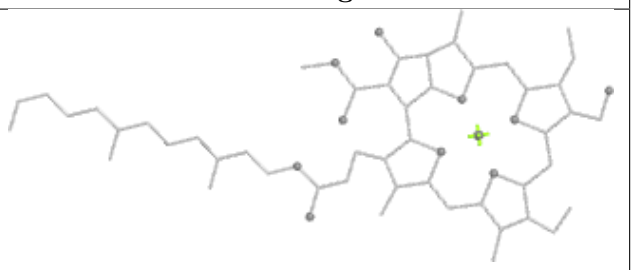
Bond lengths



Bond angles

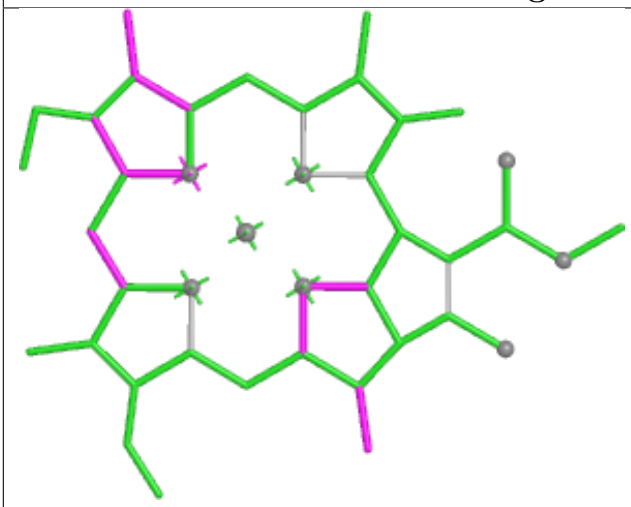


Torsions

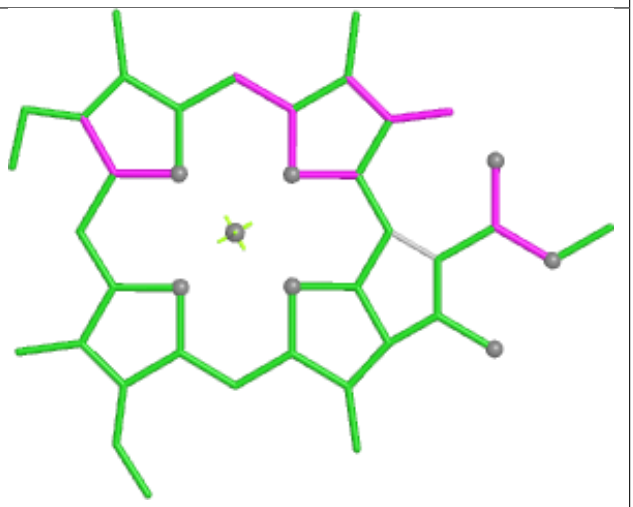


Rings

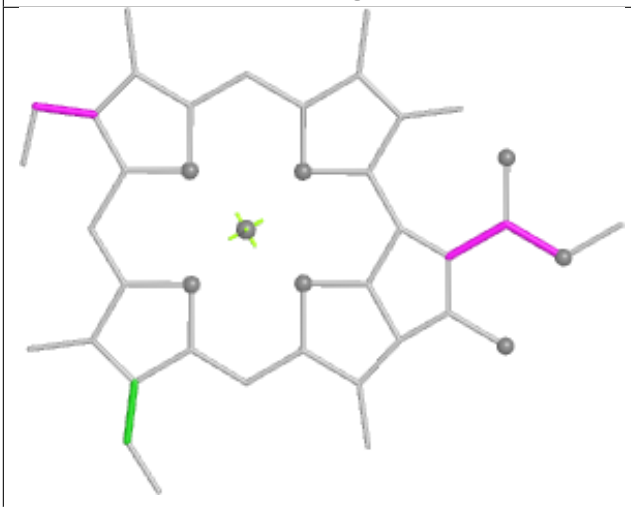
Ligand CLA 4 314



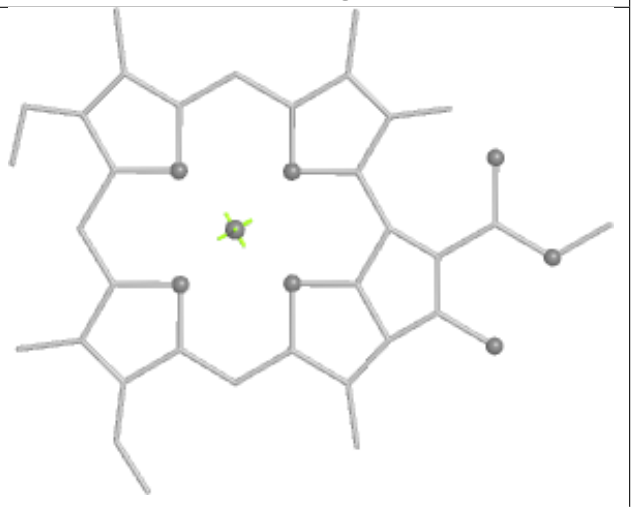
Bond lengths



Bond angles

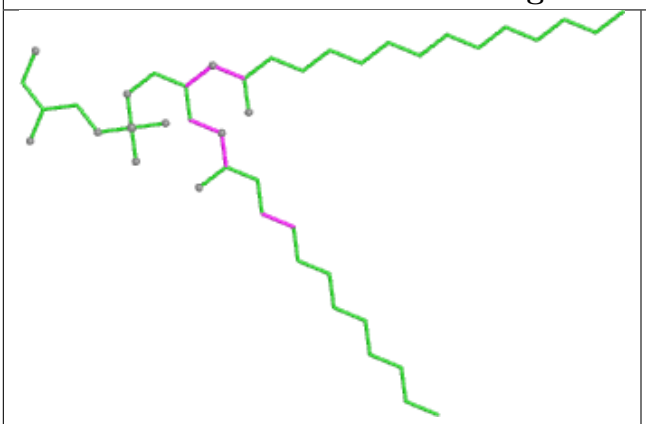


Torsions

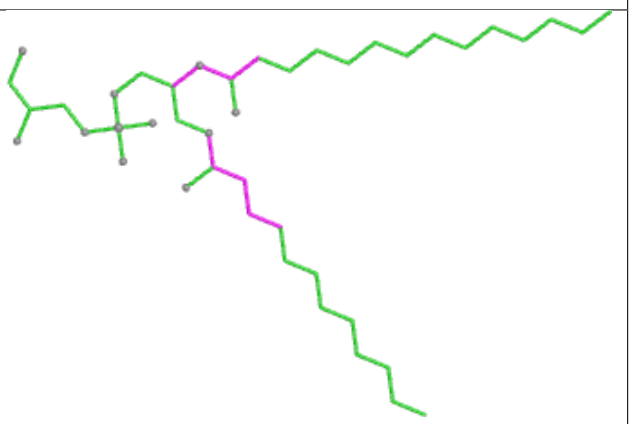


Rings

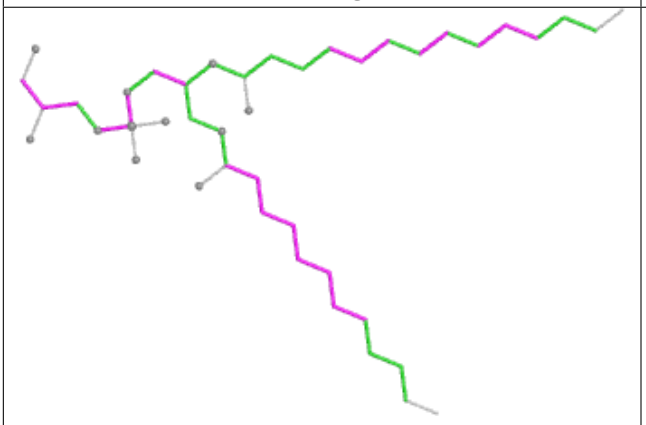
Ligand LHG 5 319



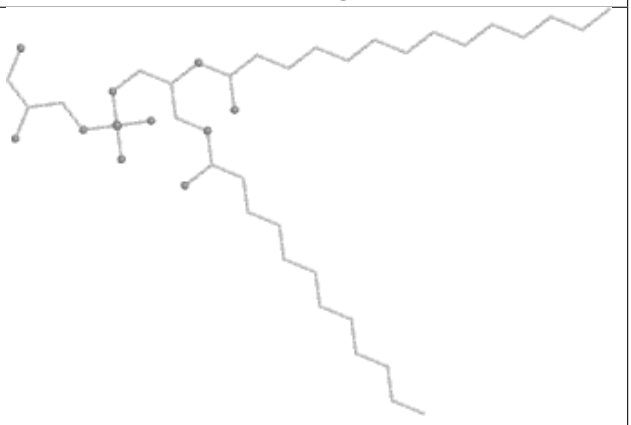
Bond lengths



Bond angles

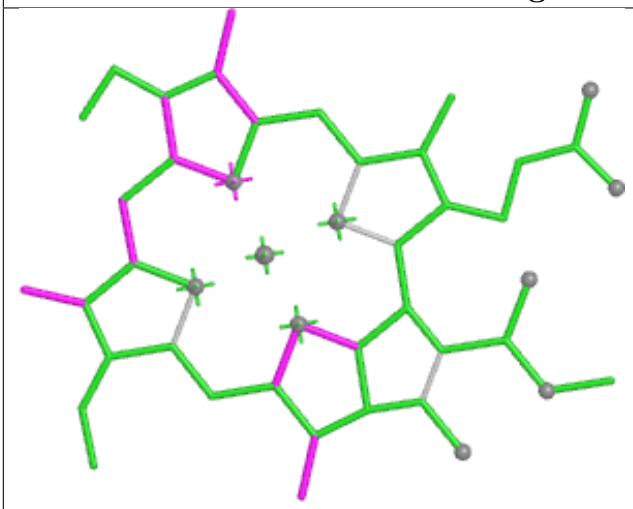


Torsions

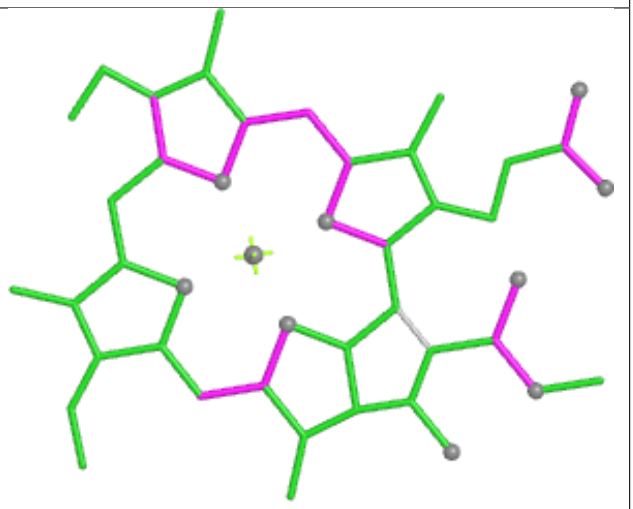


Rings

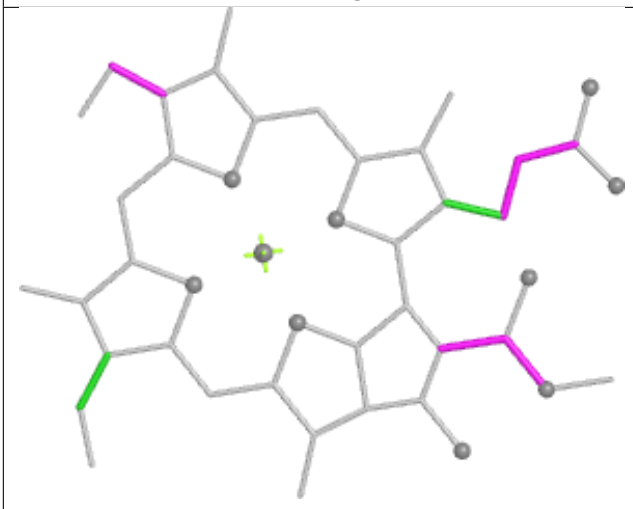
Ligand CLA 3 316



Bond lengths



Bond angles

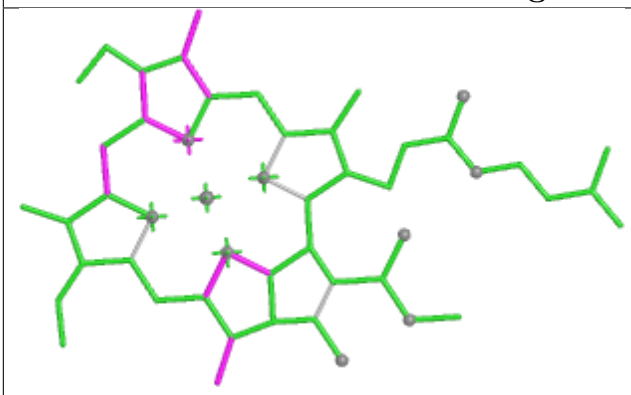


Torsions

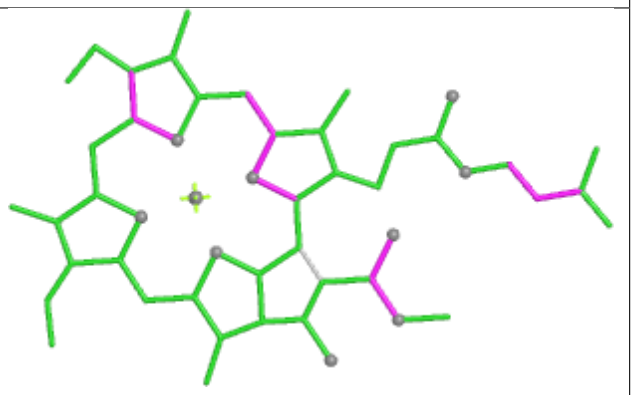


Rings

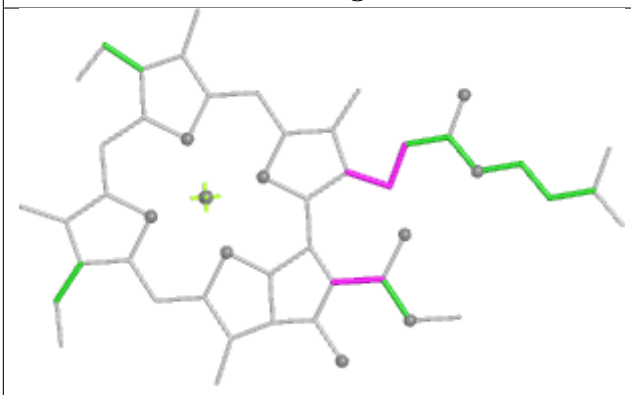
Ligand CLA 7 308



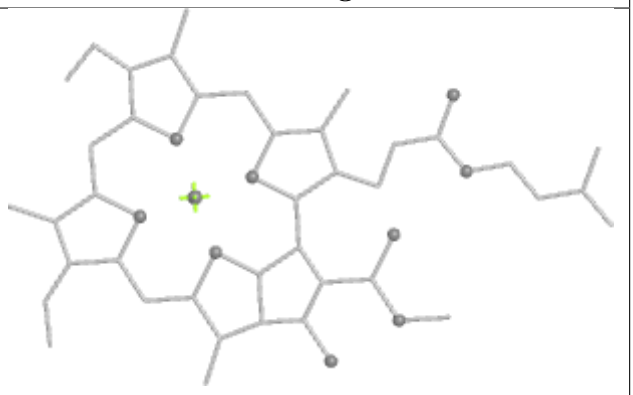
Bond lengths



Bond angles

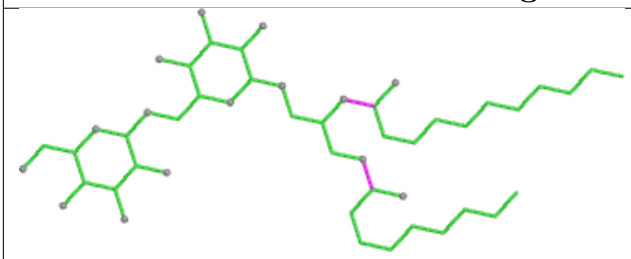


Torsions

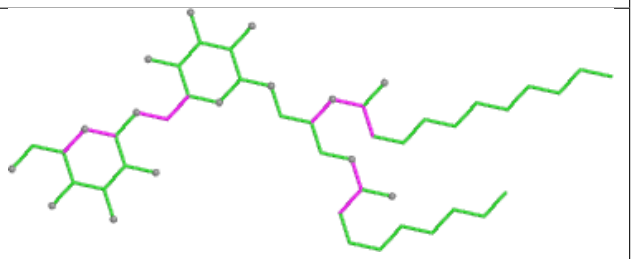


Rings

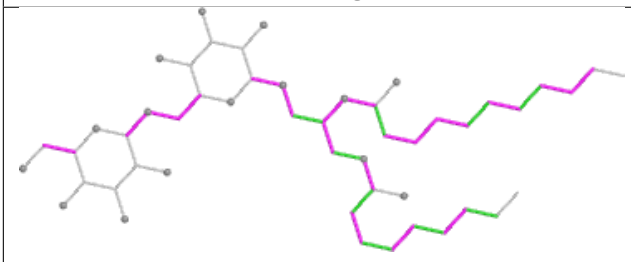
Ligand DGD C 619



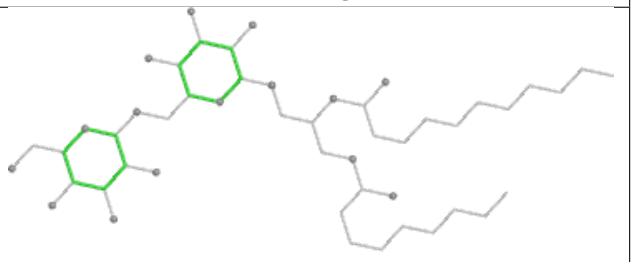
Bond lengths



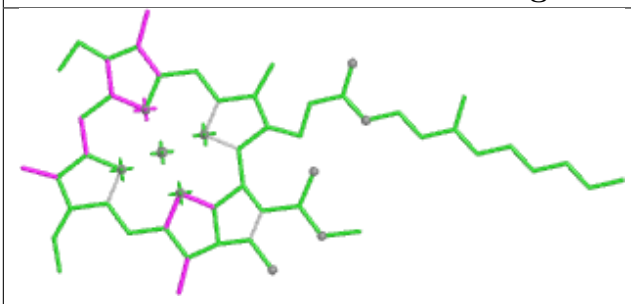
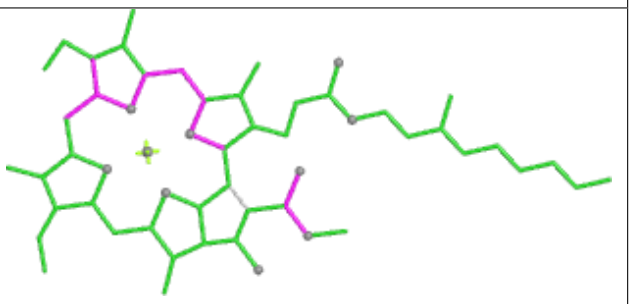
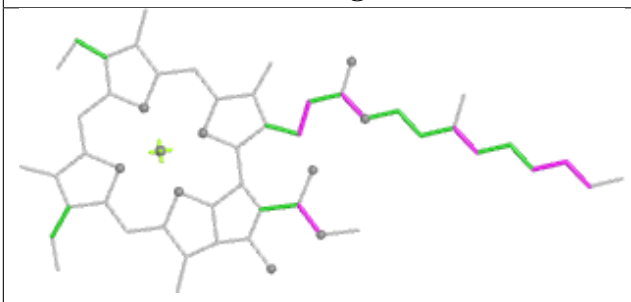
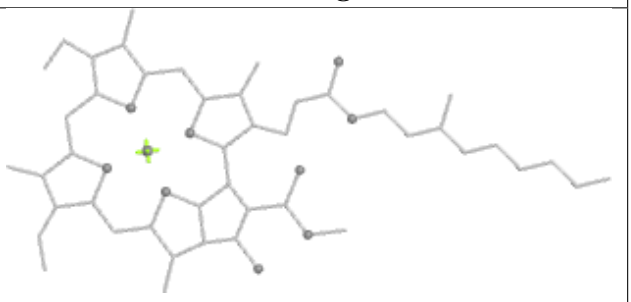
Bond angles

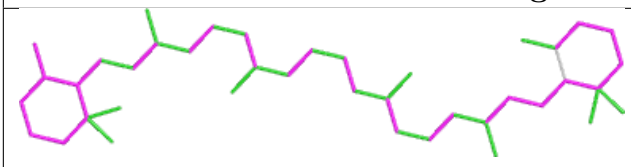
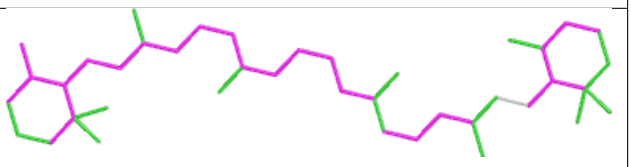
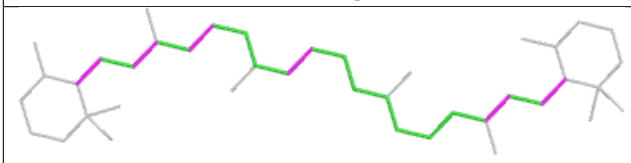
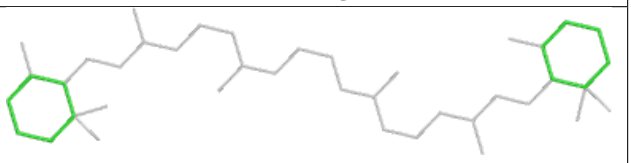


Torsions

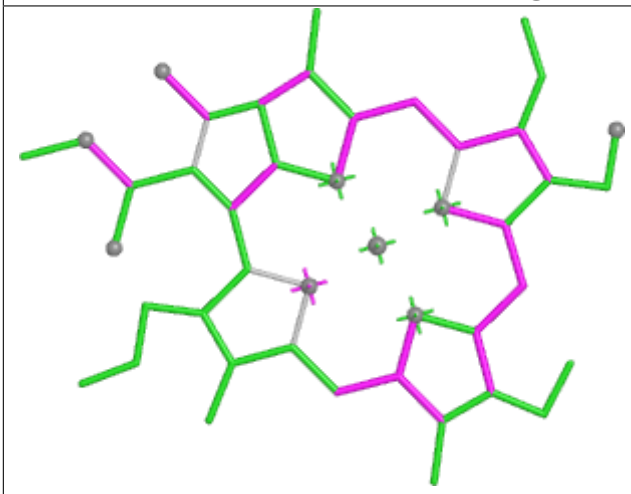


Rings

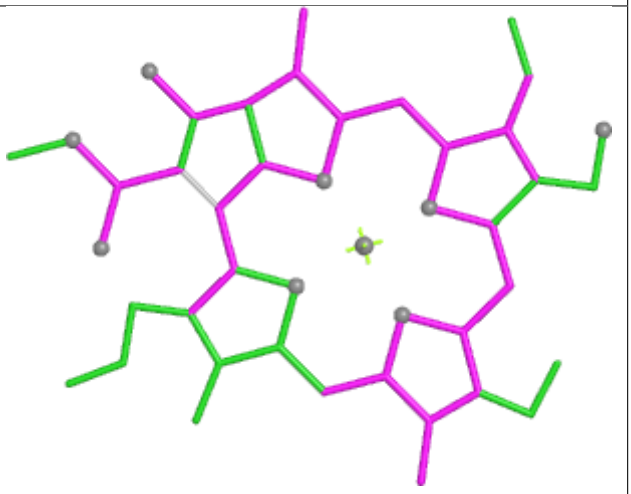
Ligand CLA s 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

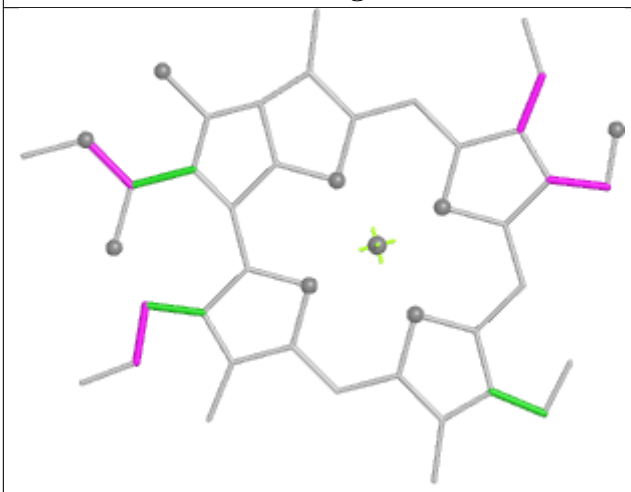
Ligand CHL 2 305



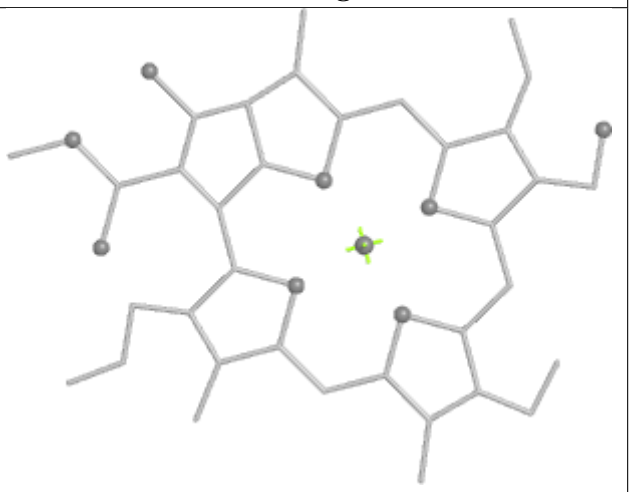
Bond lengths



Bond angles

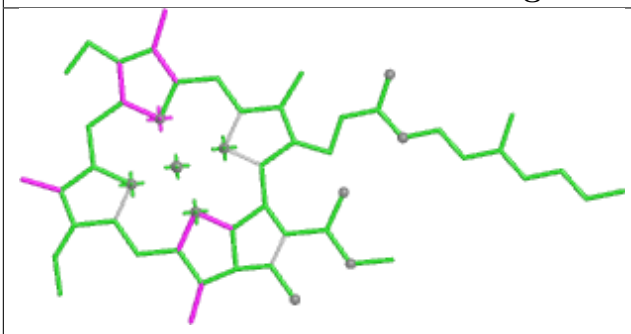


Torsions

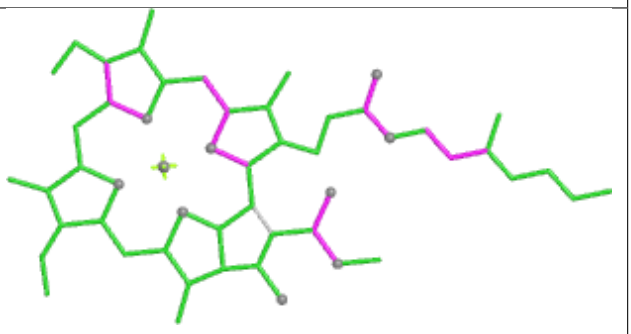


Rings

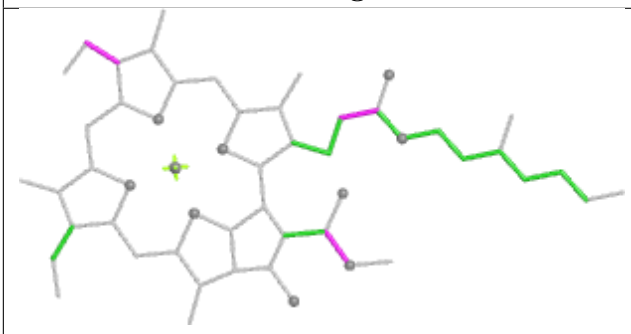
Ligand CLA Y 306



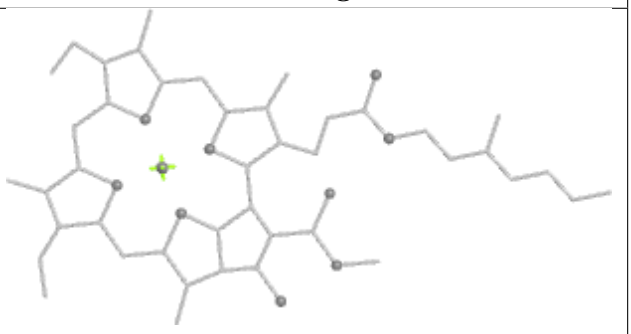
Bond lengths



Bond angles

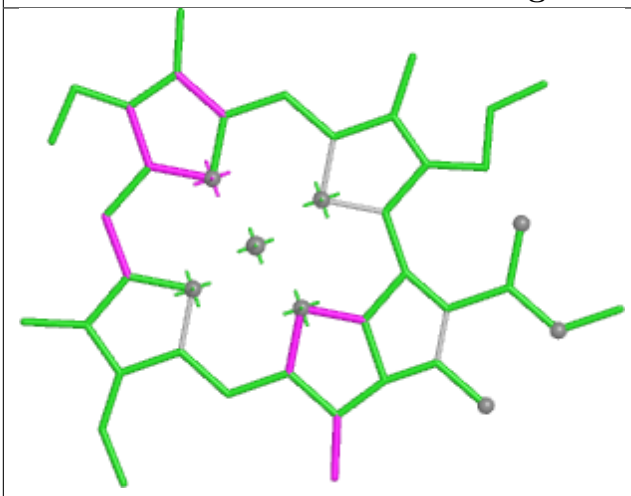


Torsions

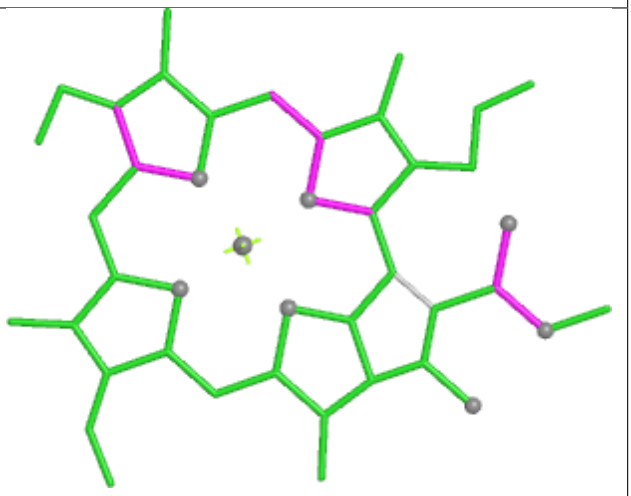


Rings

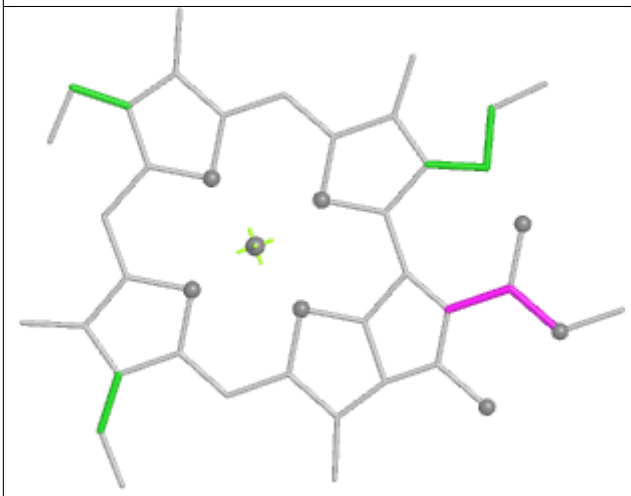
Ligand CLA 3 307



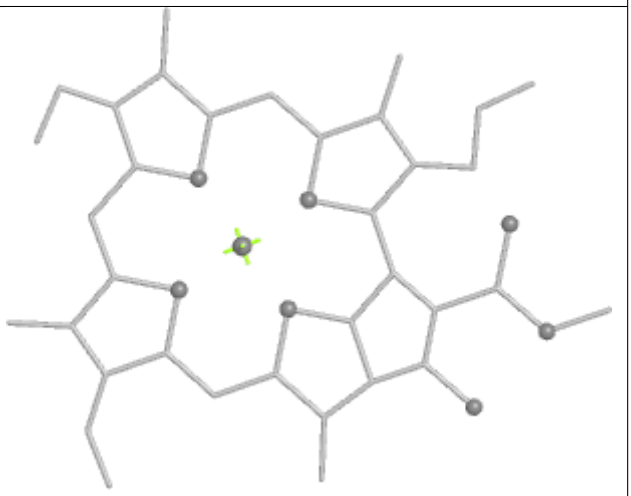
Bond lengths



Bond angles

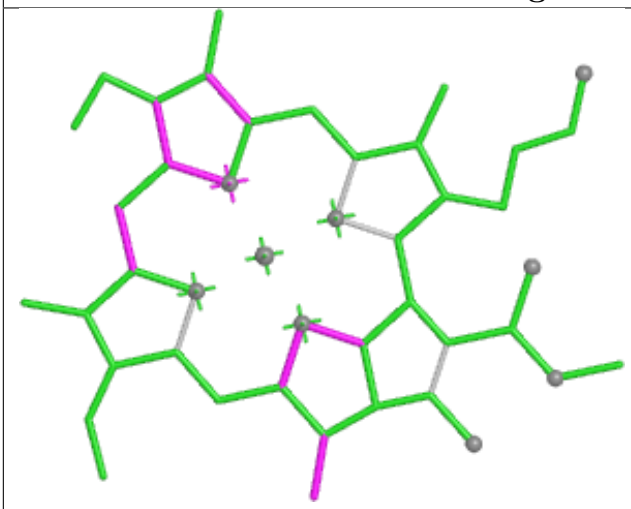


Torsions

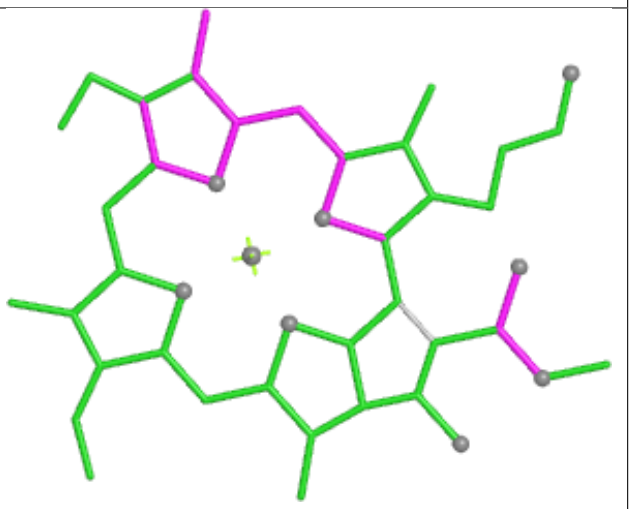


Rings

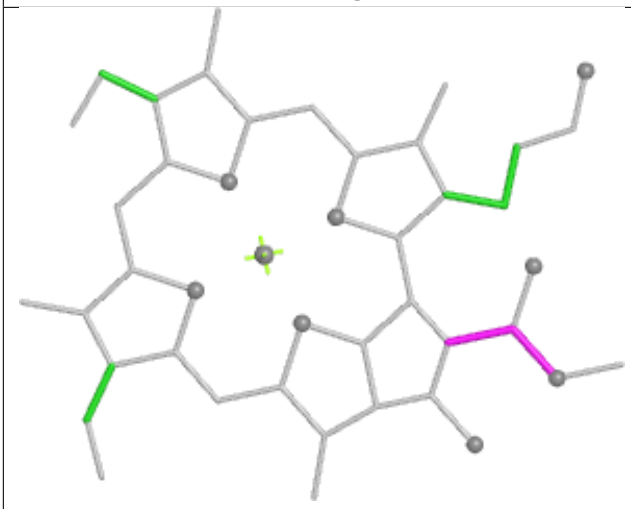
Ligand CLA 4 306



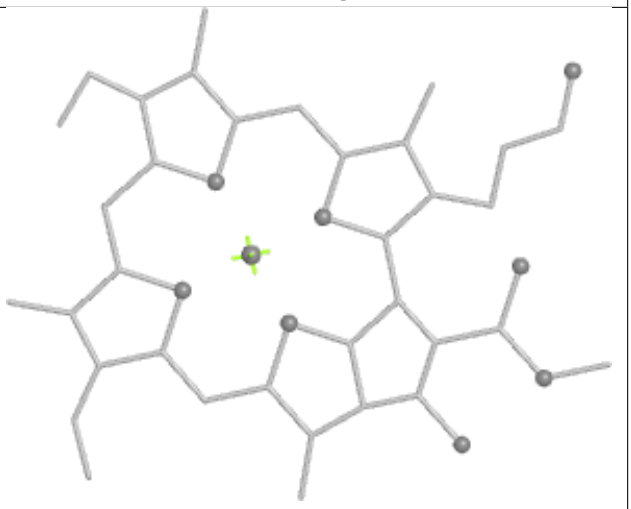
Bond lengths



Bond angles

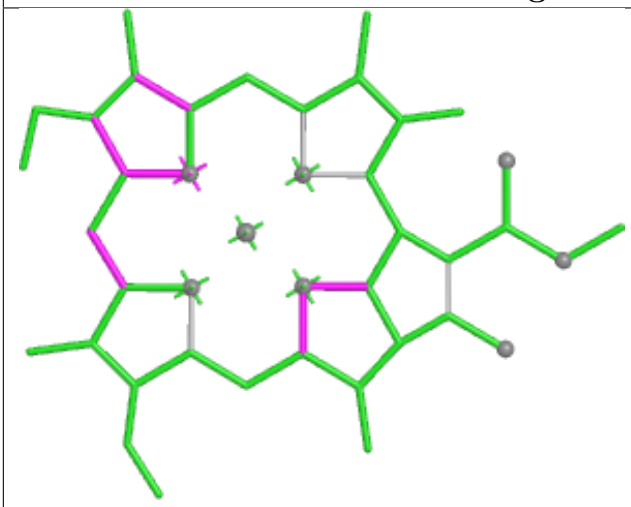


Torsions

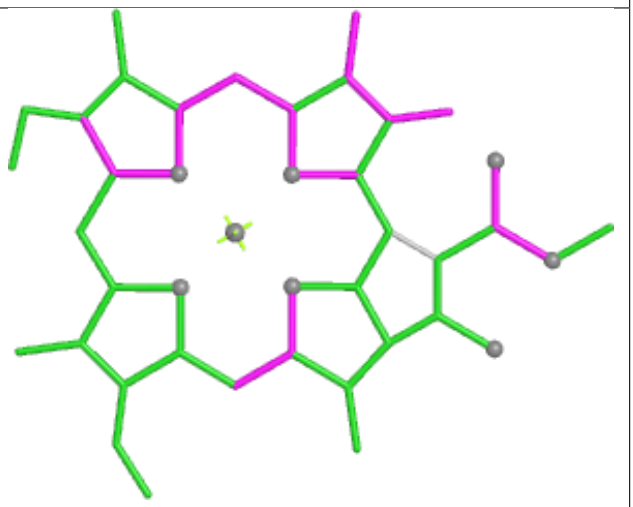


Rings

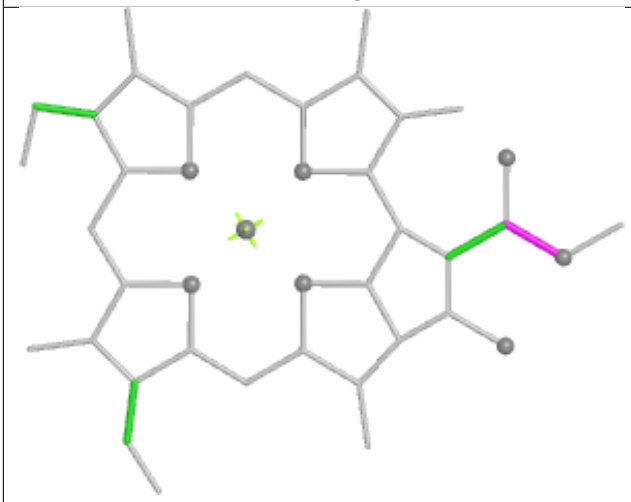
Ligand CLA 6 313



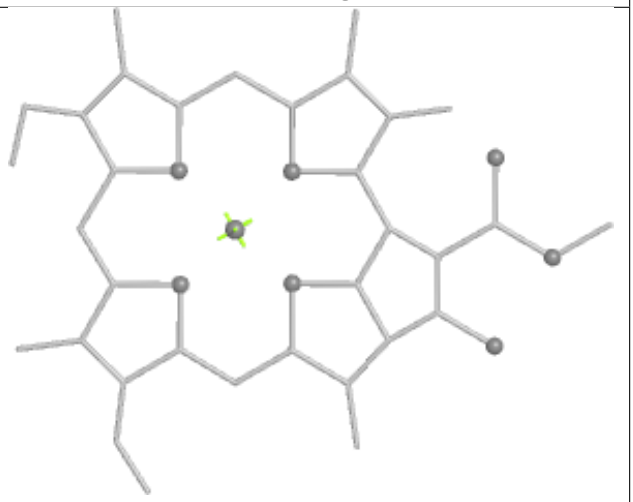
Bond lengths



Bond angles

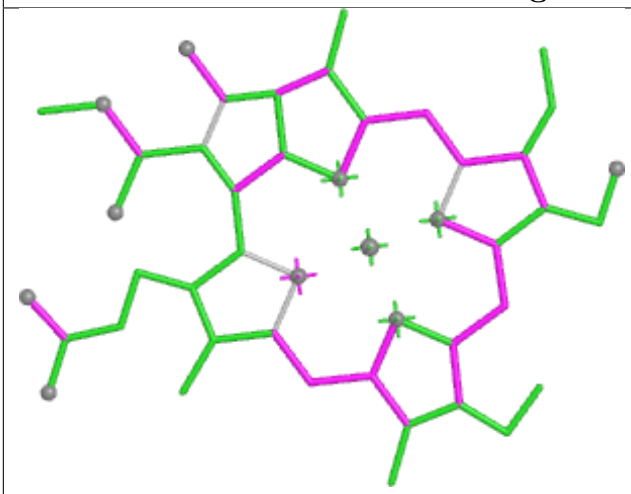


Torsions

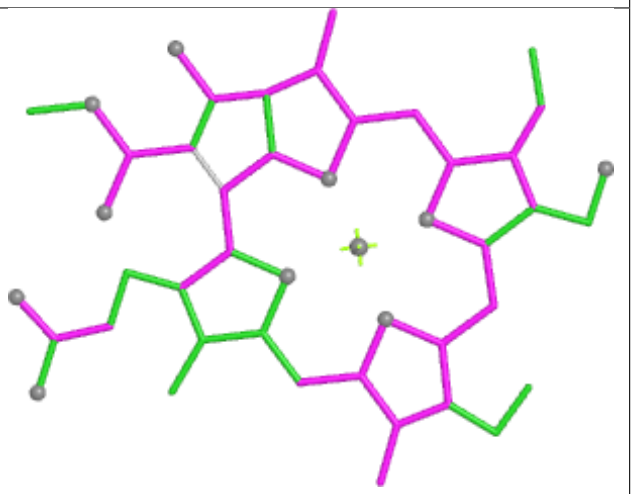


Rings

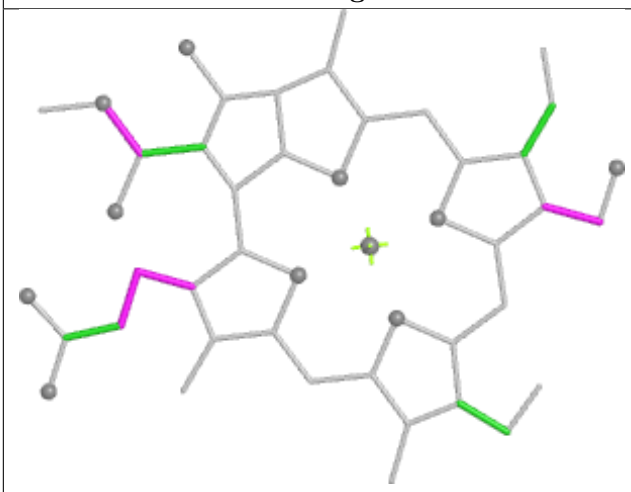
Ligand CHL s 408



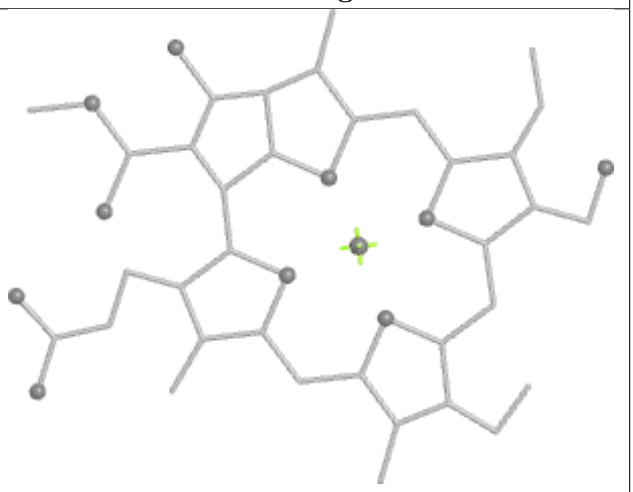
Bond lengths



Bond angles

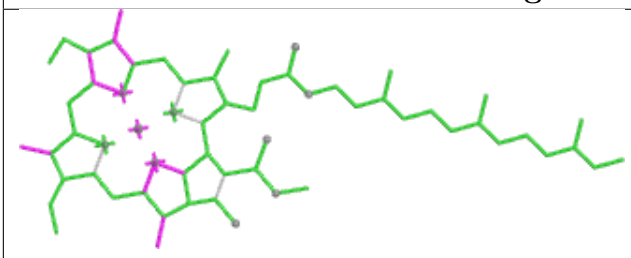


Torsions

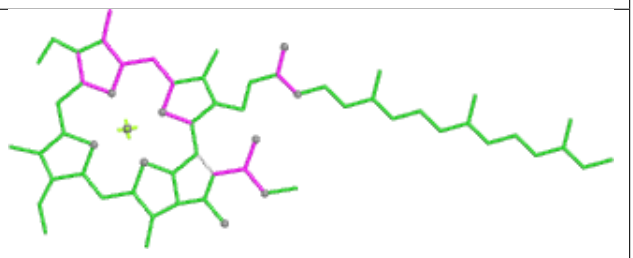


Rings

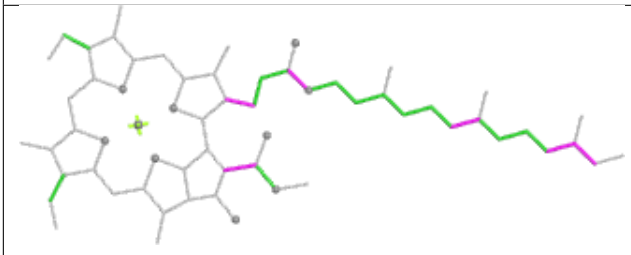
Ligand CLA C 608



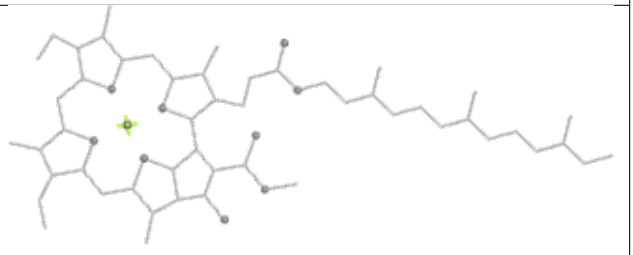
Bond lengths



Bond angles

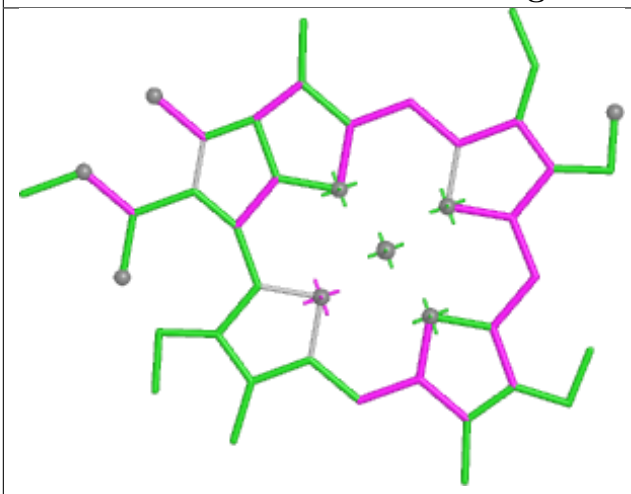


Torsions

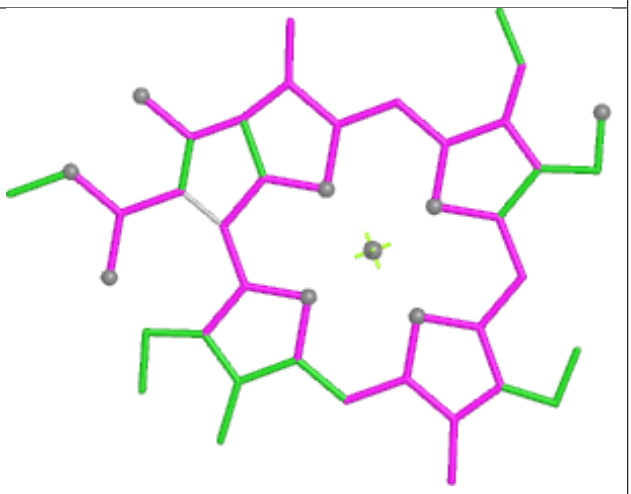


Rings

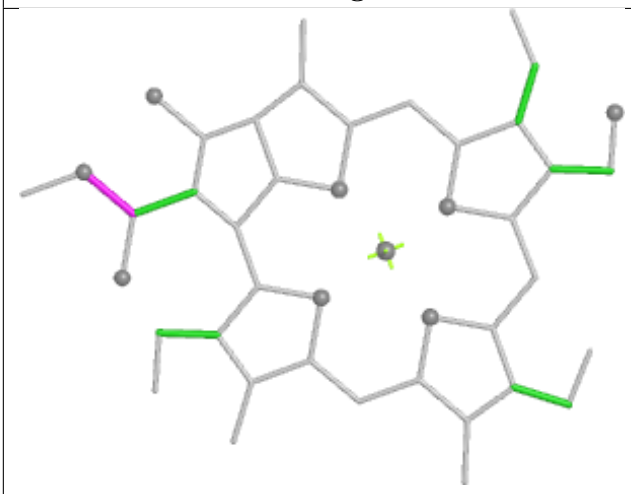
Ligand CHL 1 308



Bond lengths



Bond angles

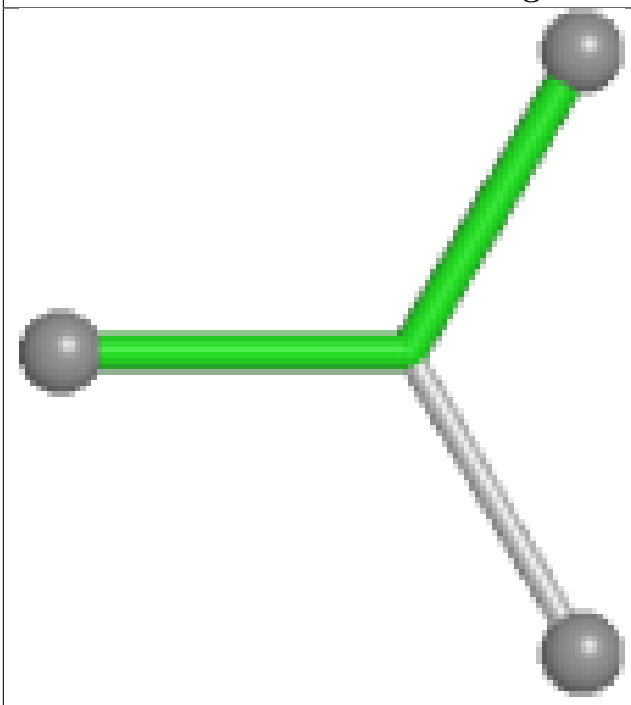


Torsions

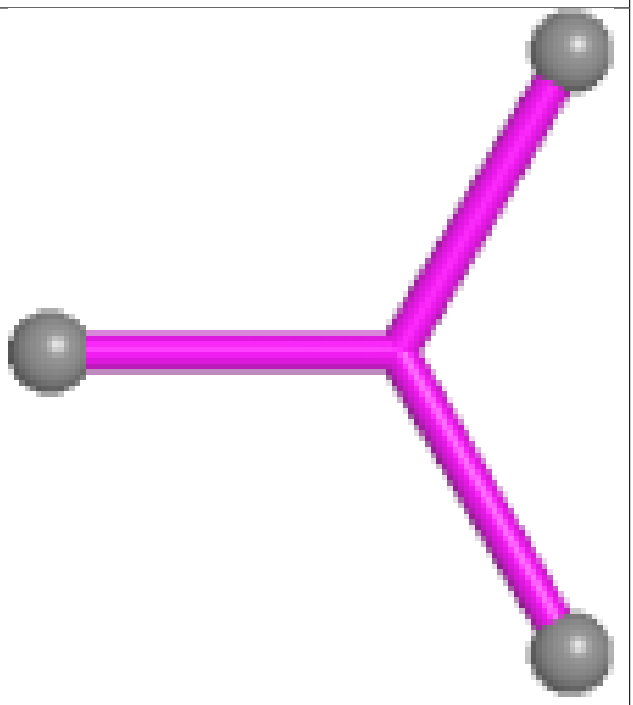


Rings

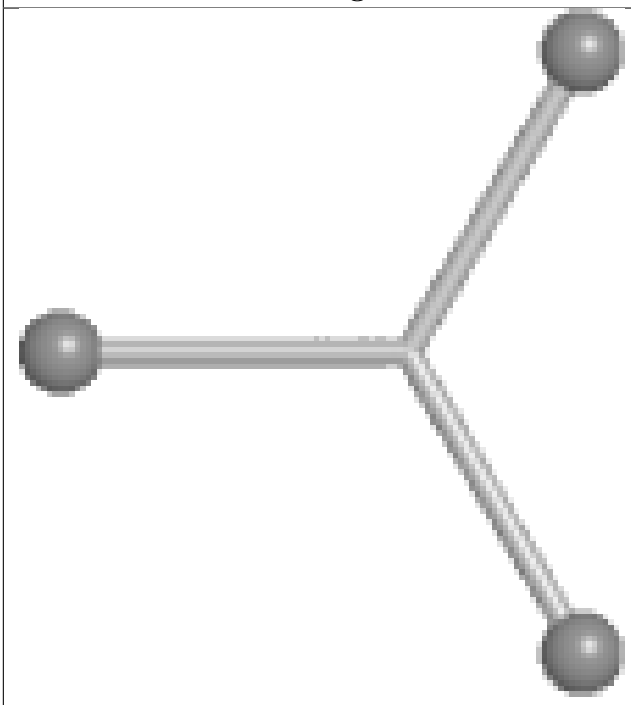
Ligand BCT A 611



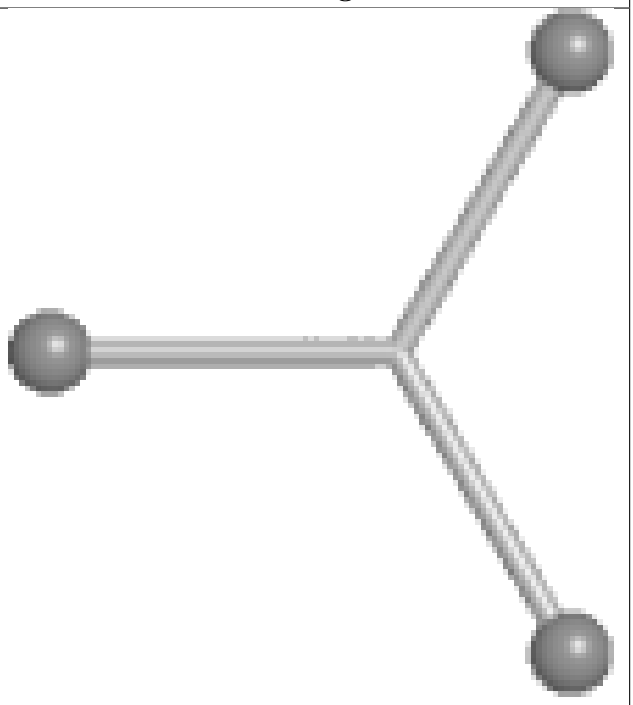
Bond lengths



Bond angles

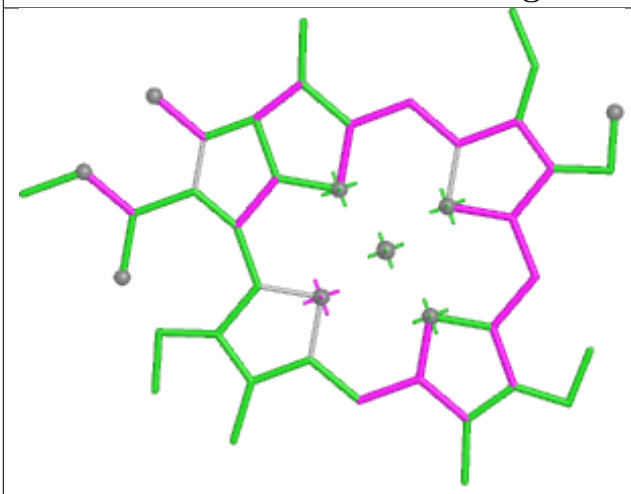


Torsions

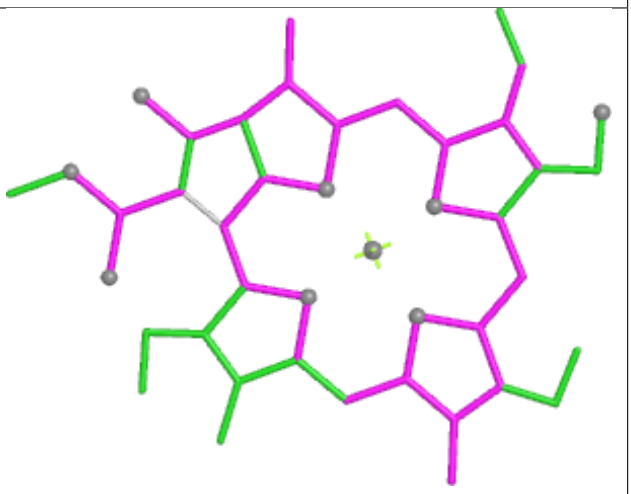


Rings

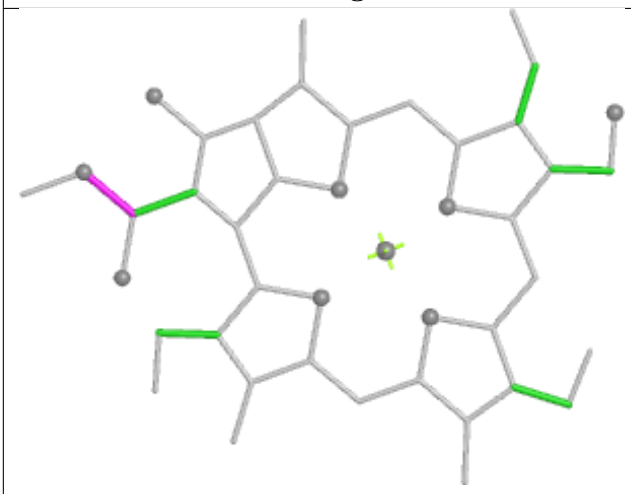
Ligand CHL G 309



Bond lengths



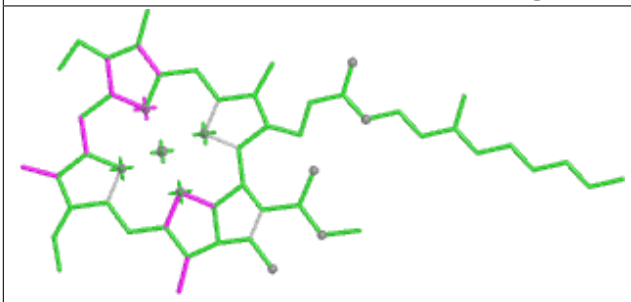
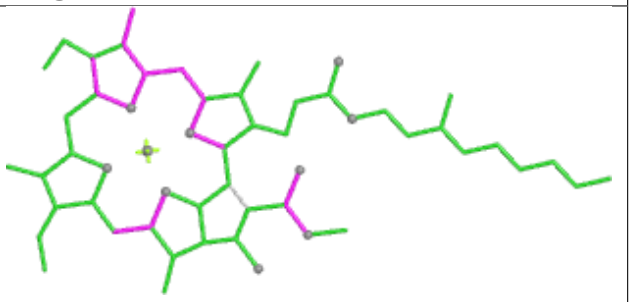
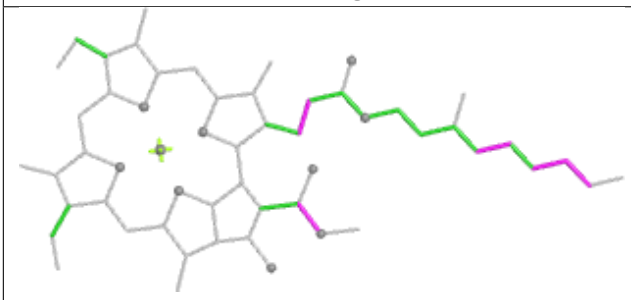
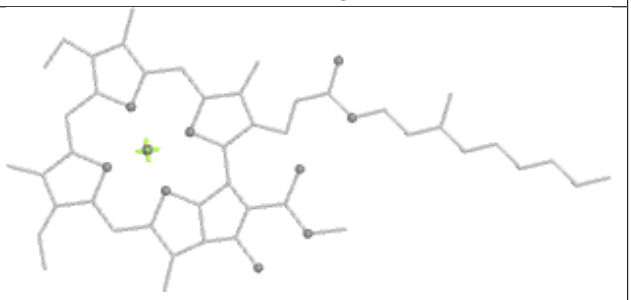
Bond angles

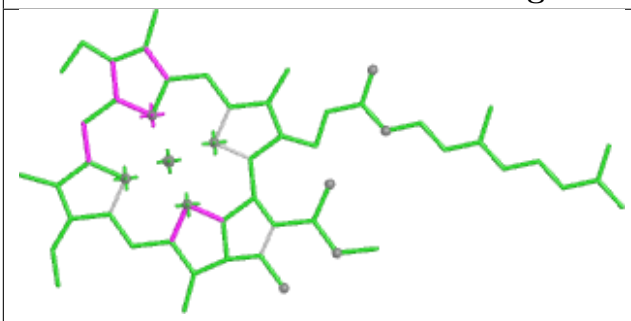
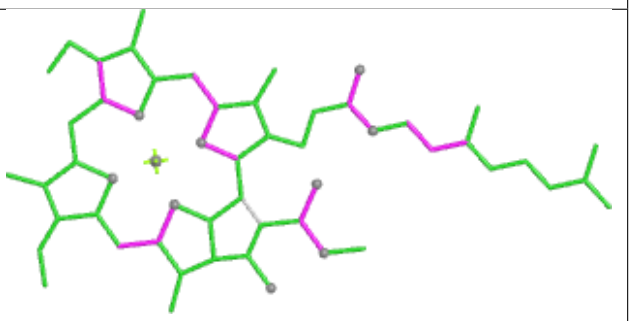
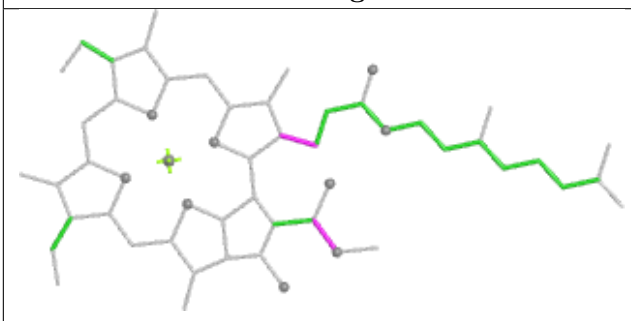
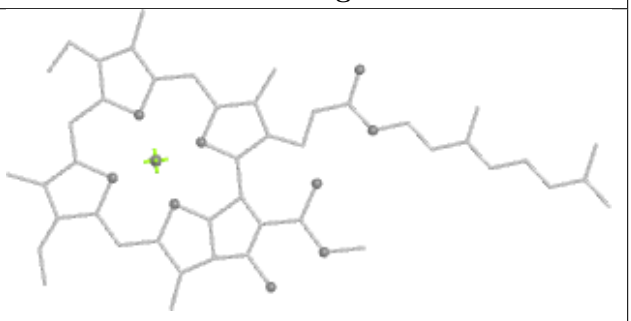


Torsions

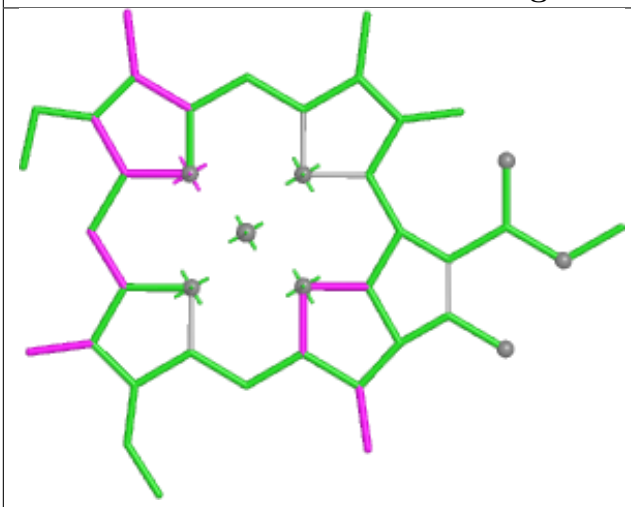


Rings

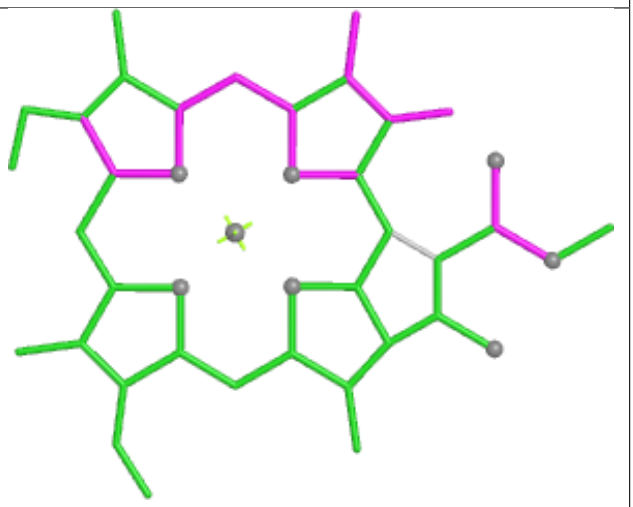
Ligand CLA g 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

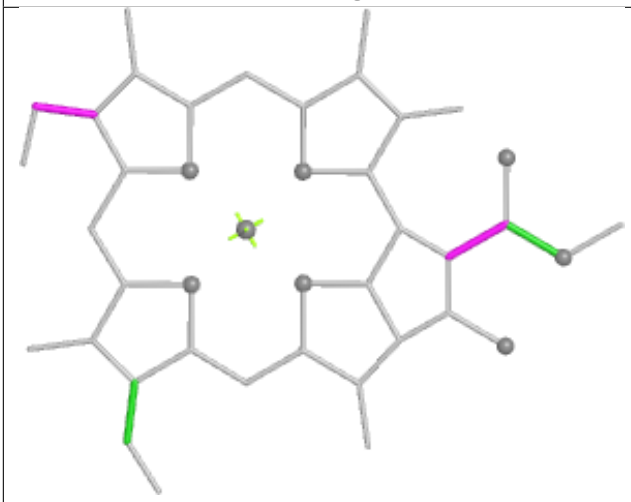
Ligand CLA r 305



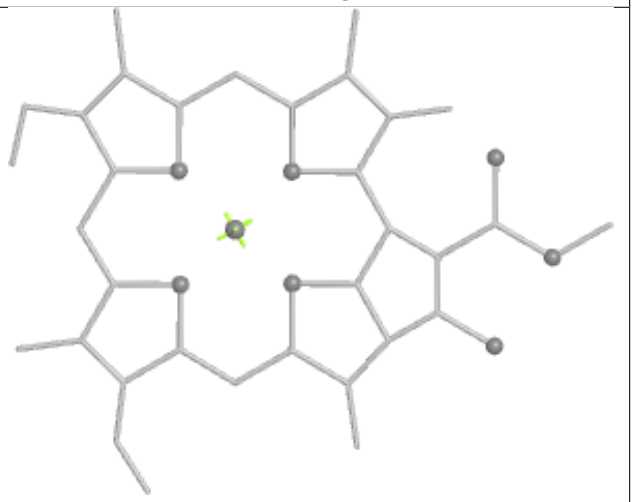
Bond lengths



Bond angles

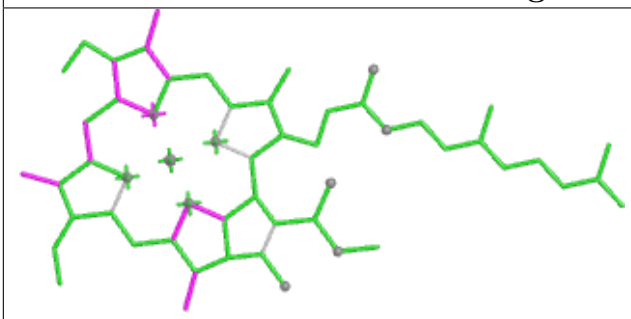


Torsions

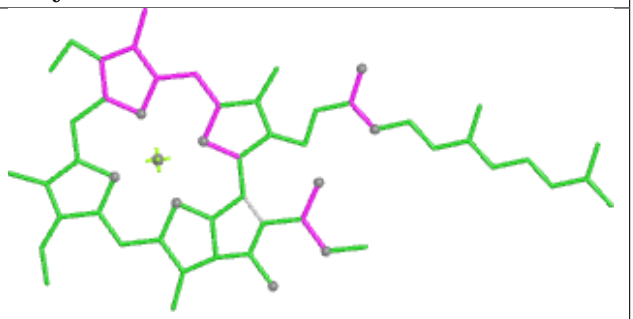


Rings

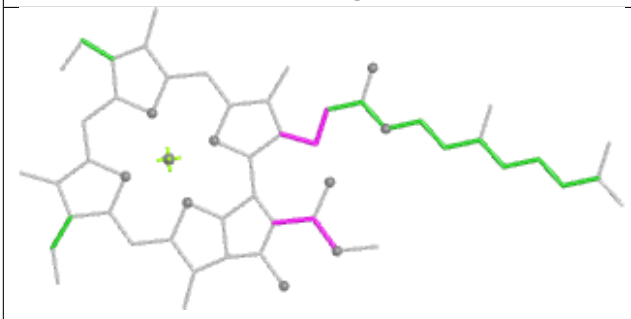
Ligand CLA y 314



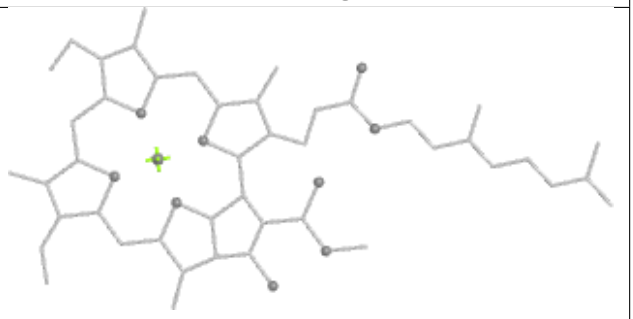
Bond lengths



Bond angles

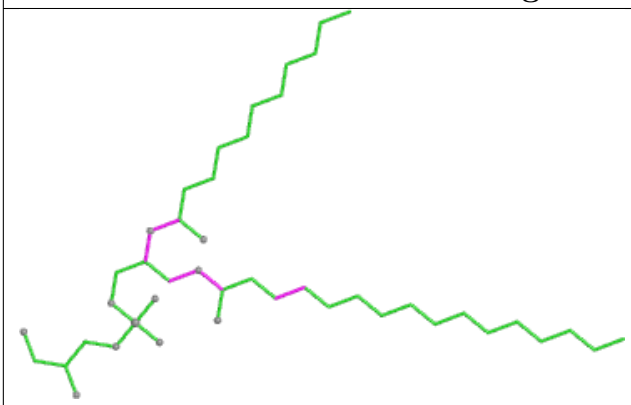


Torsions

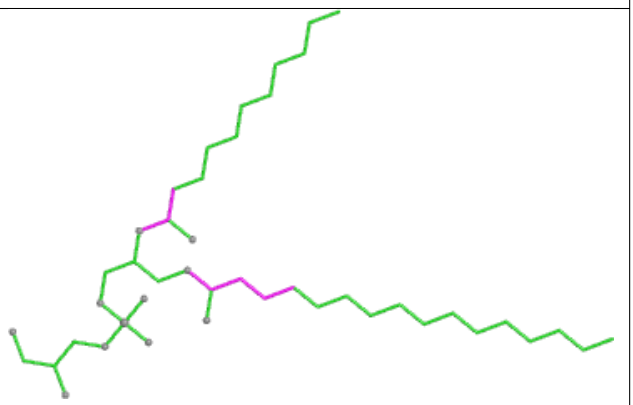


Rings

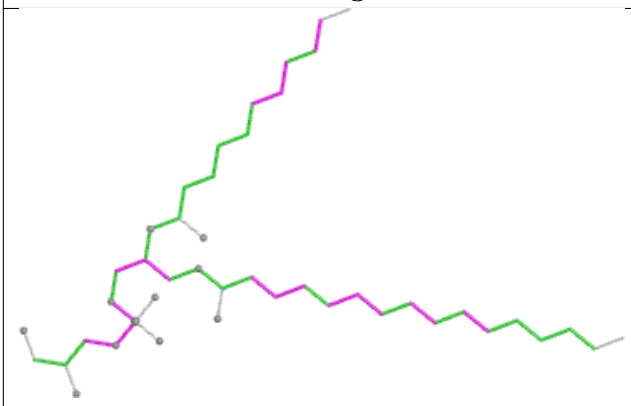
Ligand LHG A 612



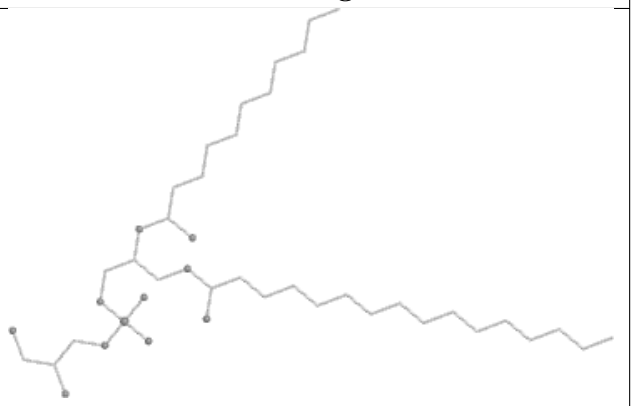
Bond lengths



Bond angles

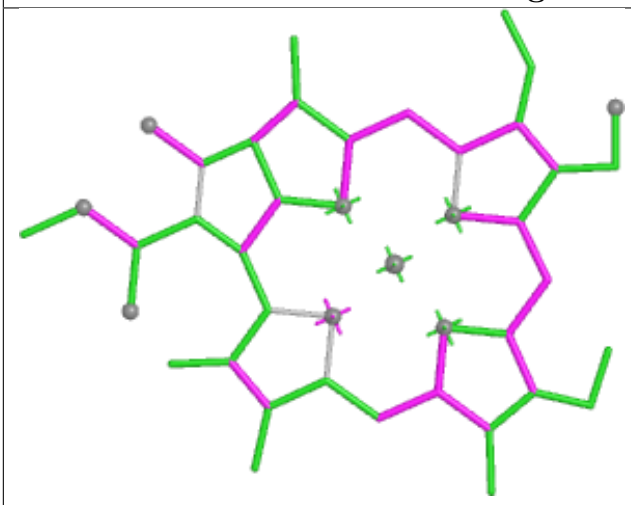


Torsions

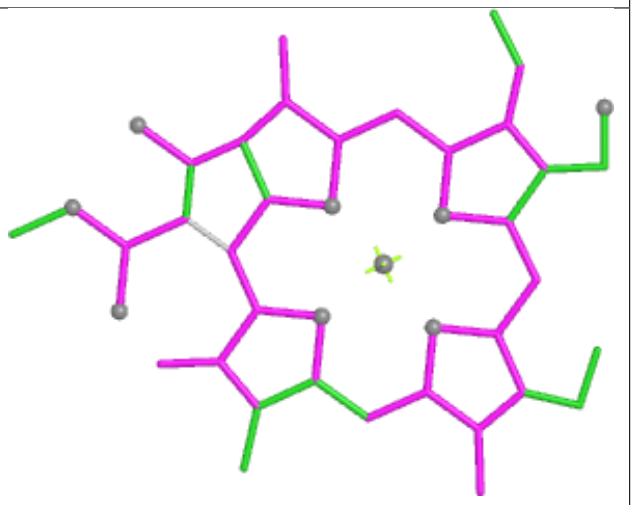


Rings

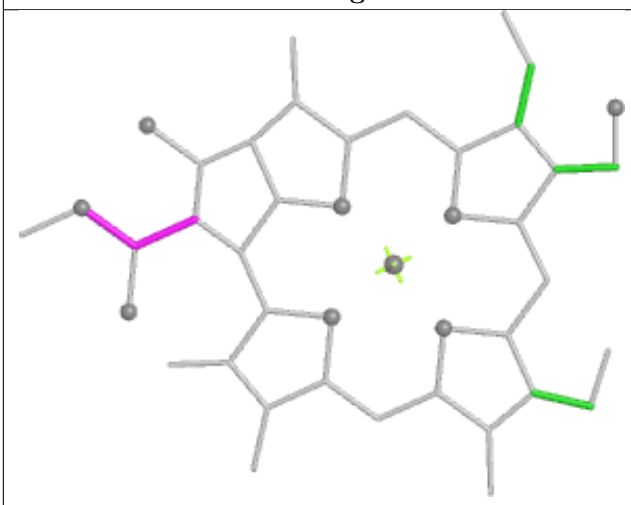
Ligand CHL 2 318



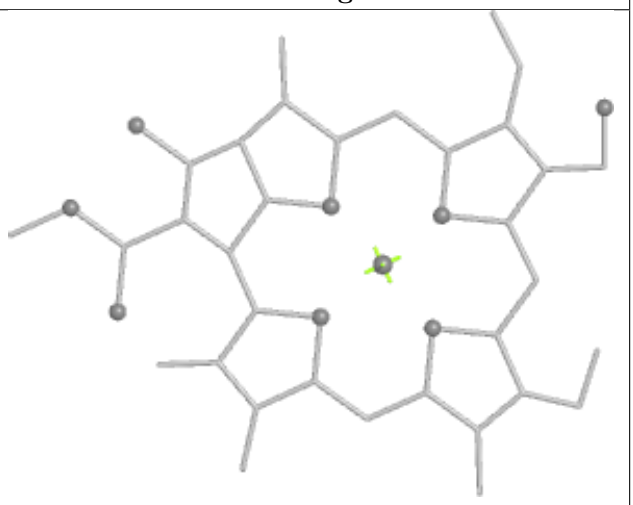
Bond lengths



Bond angles

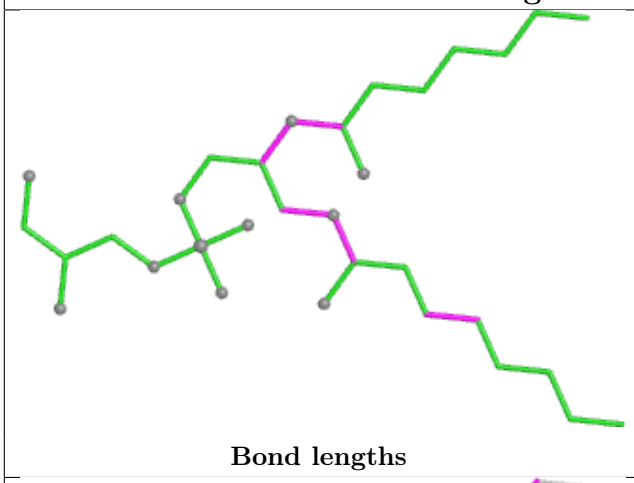


Torsions

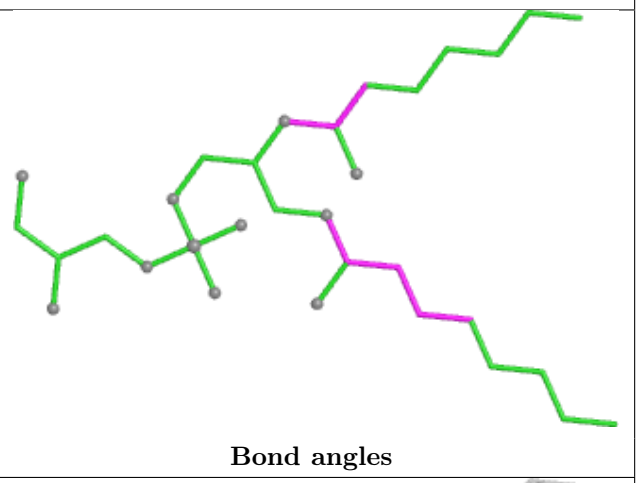


Rings

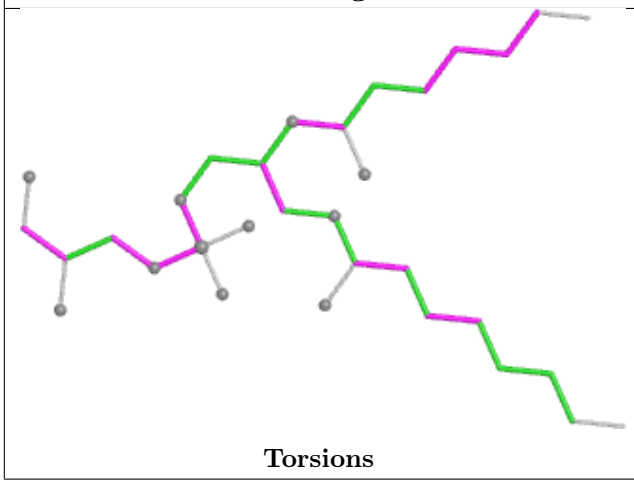
Ligand LHG C 617



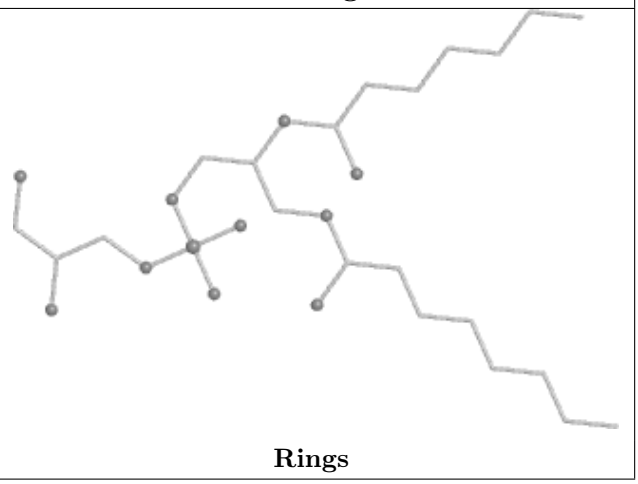
Bond lengths



Bond angles

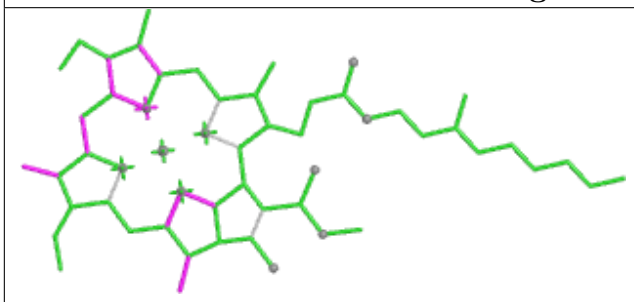


Torsions

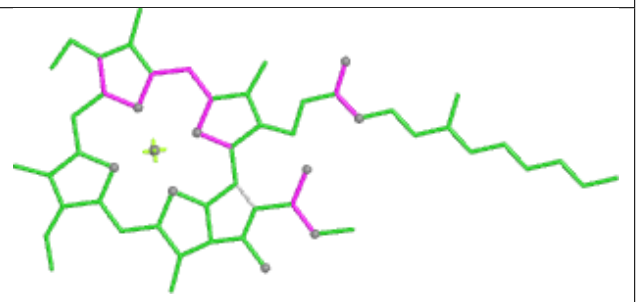


Rings

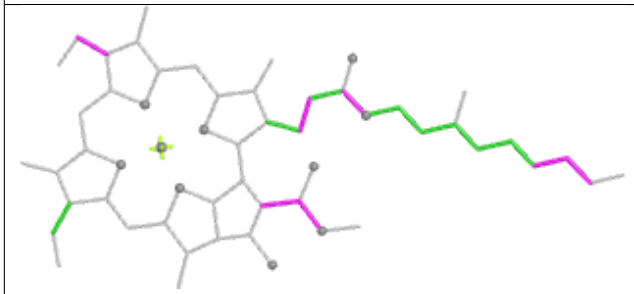
Ligand CLA 9 316



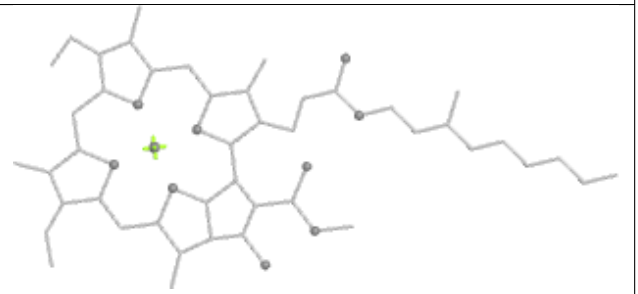
Bond lengths



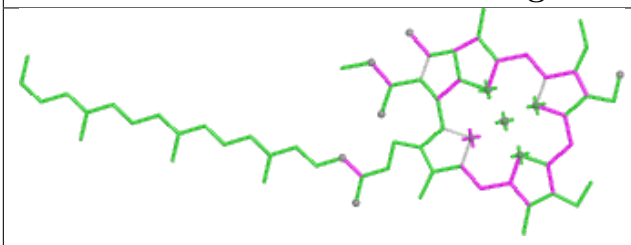
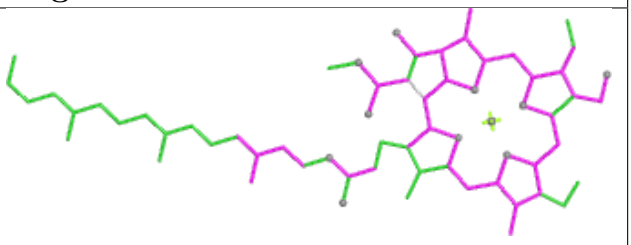
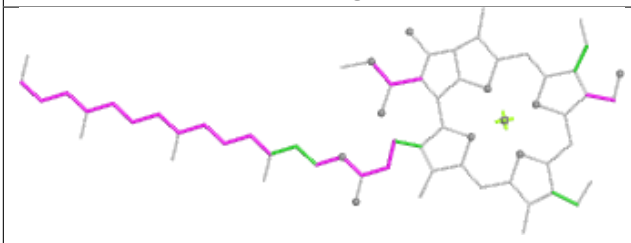
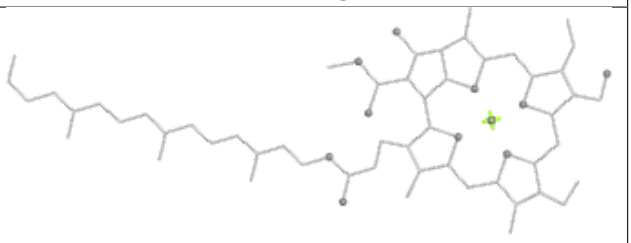
Bond angles

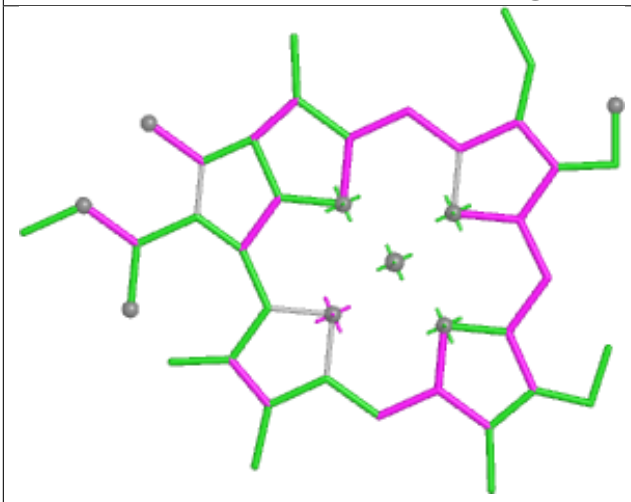
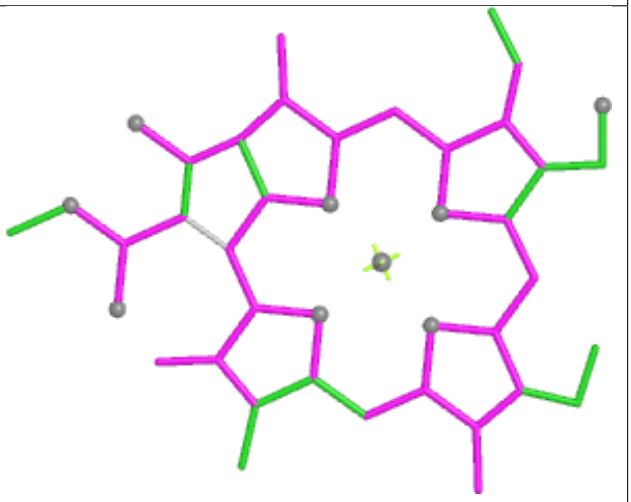
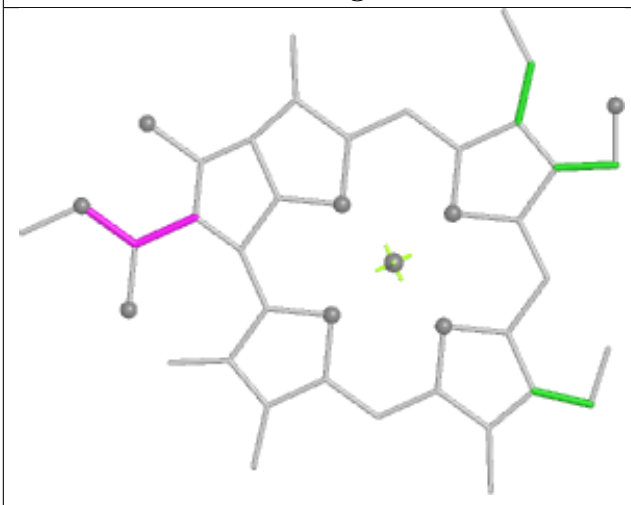
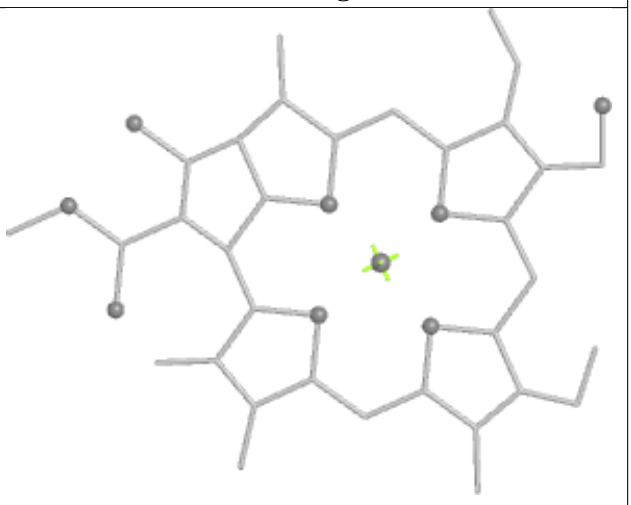


Torsions

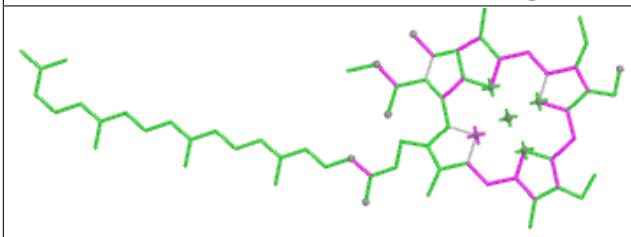


Rings

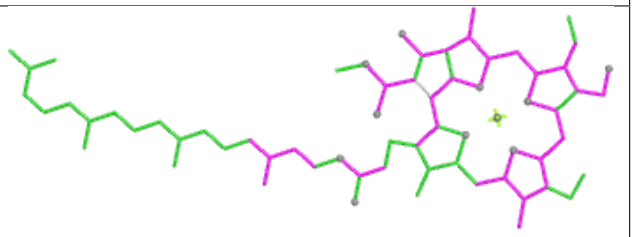
Ligand CHL g 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL u 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

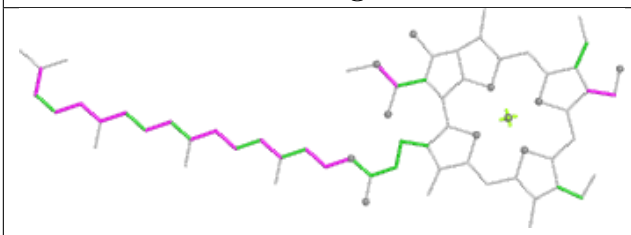
Ligand CHL Y 312



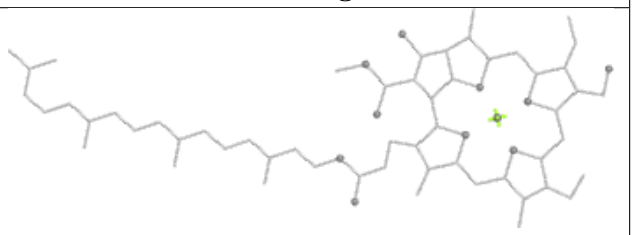
Bond lengths



Bond angles

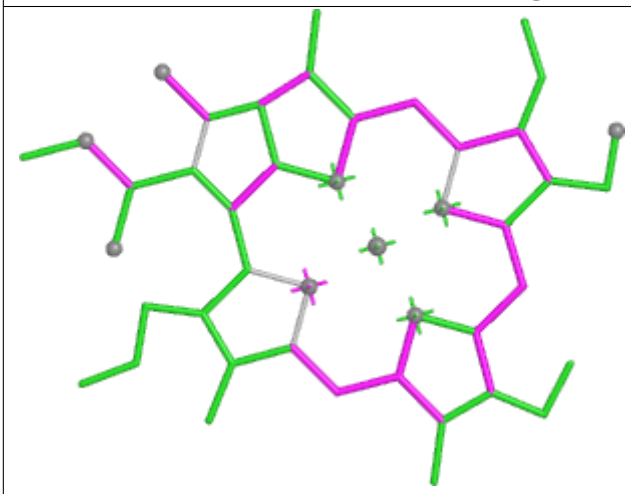


Torsions

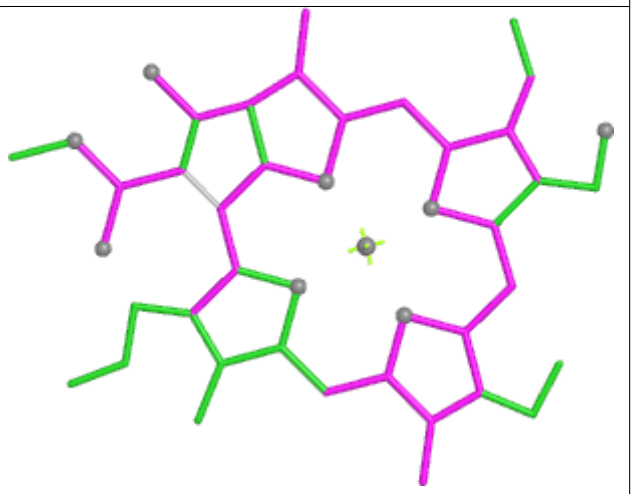


Rings

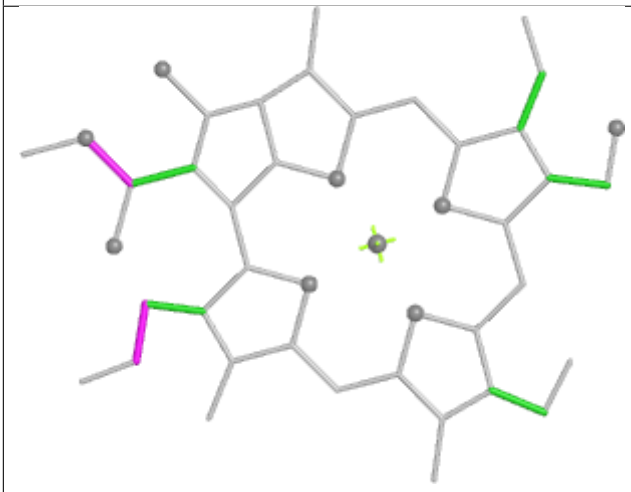
Ligand CHL 1 311



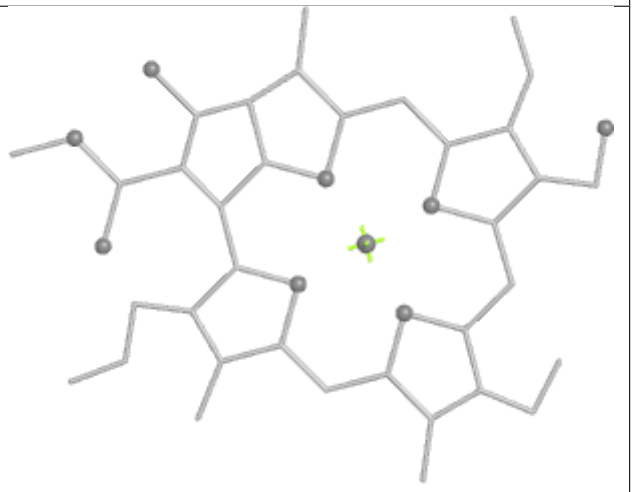
Bond lengths



Bond angles

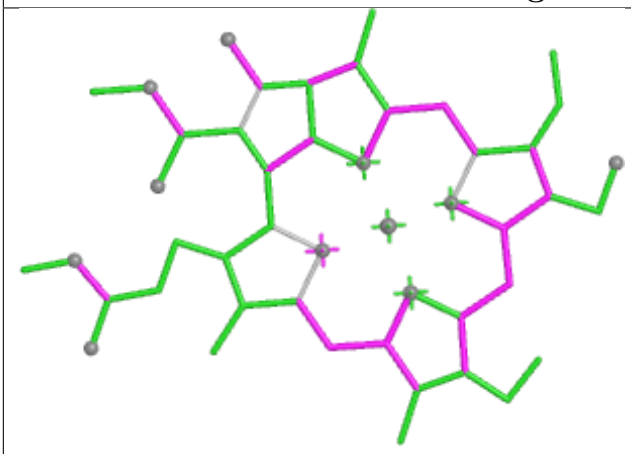


Torsions

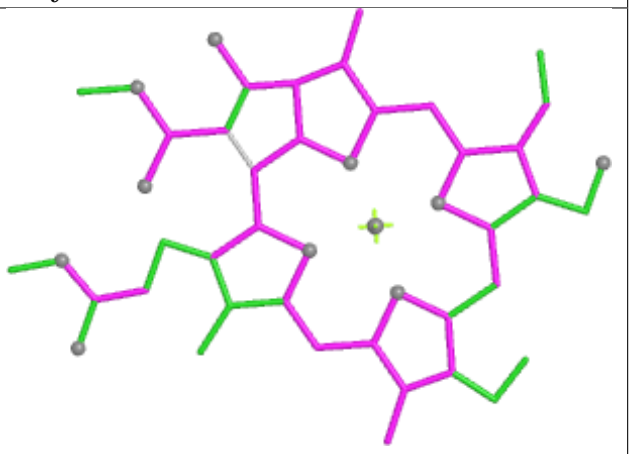


Rings

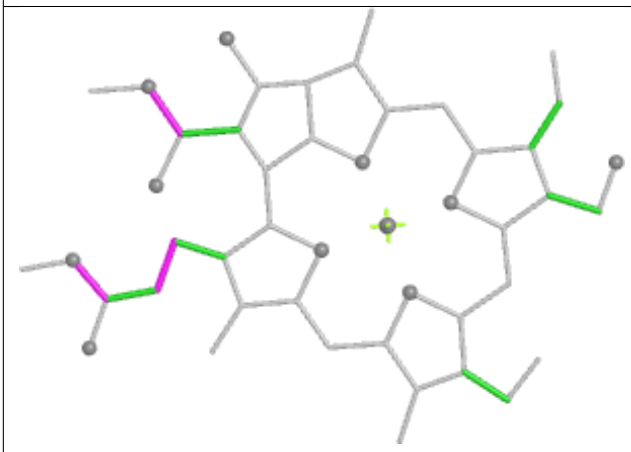
Ligand CHL y 310



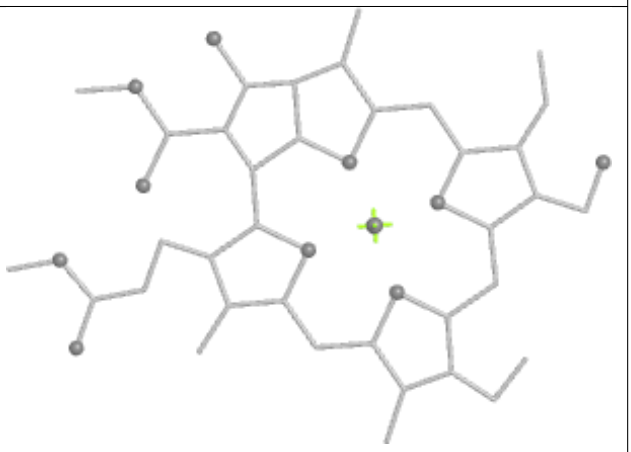
Bond lengths



Bond angles

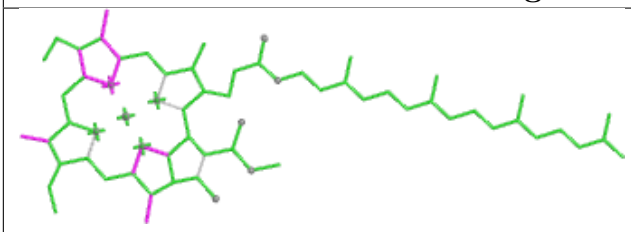


Torsions

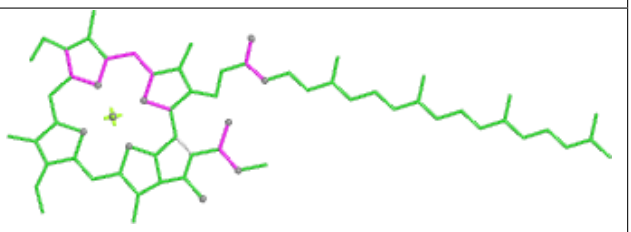


Rings

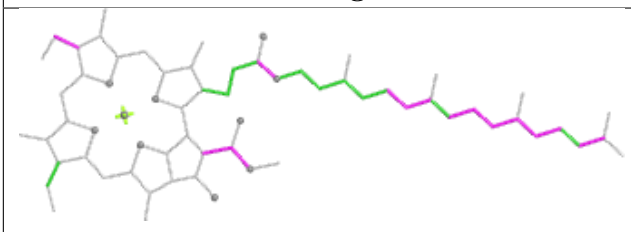
Ligand CLA C 602



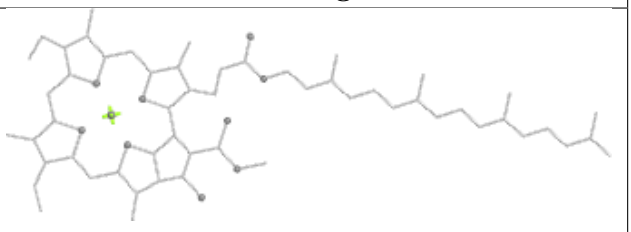
Bond lengths



Bond angles

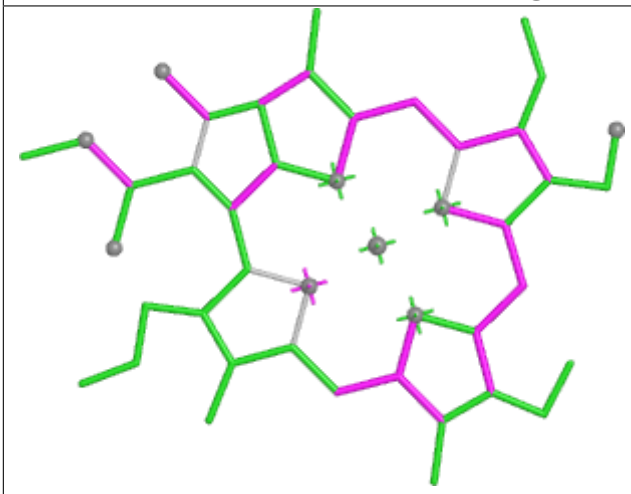


Torsions

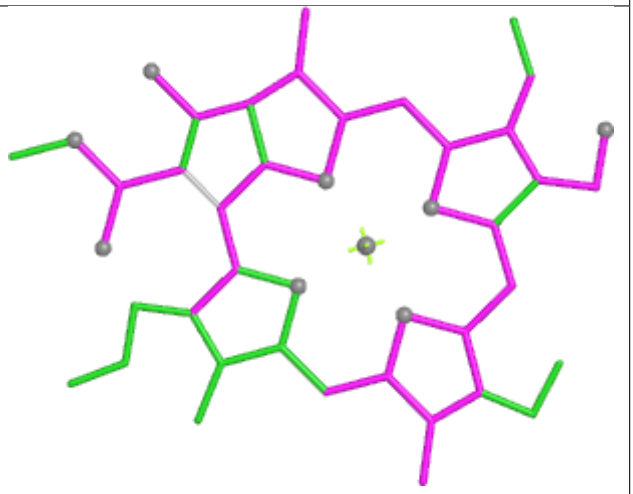


Rings

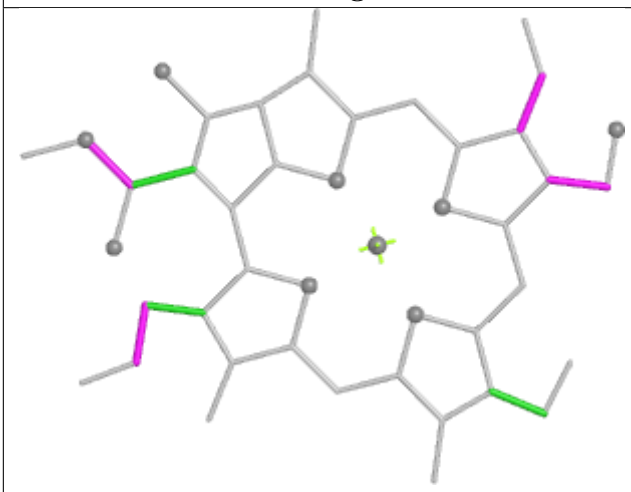
Ligand CHL 5 305



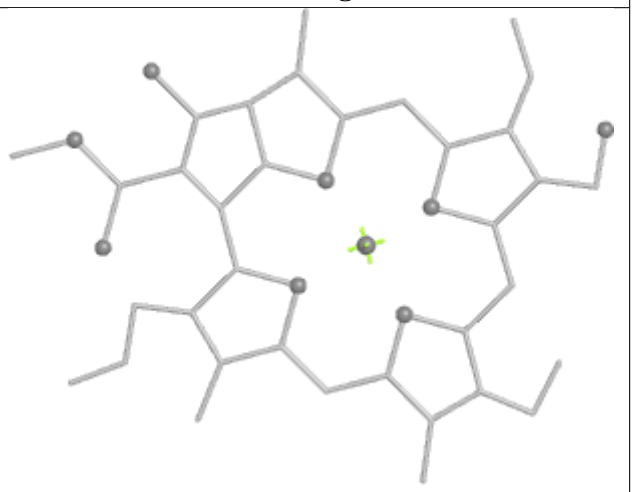
Bond lengths



Bond angles

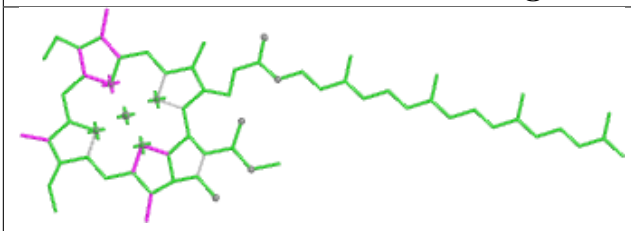


Torsions

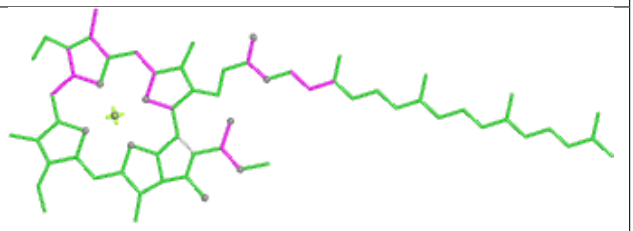


Rings

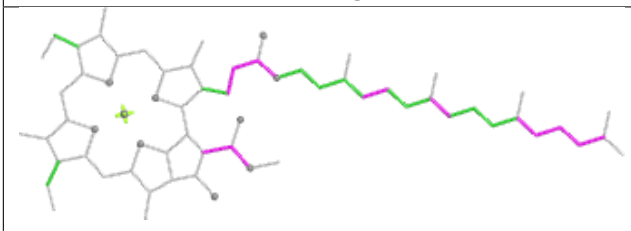
Ligand CLA B 606



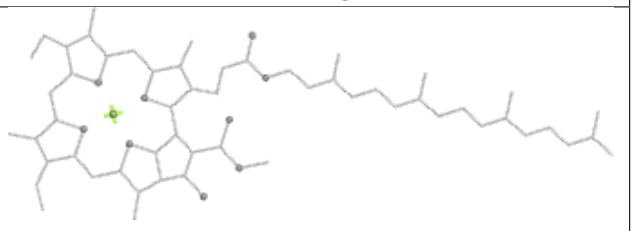
Bond lengths



Bond angles

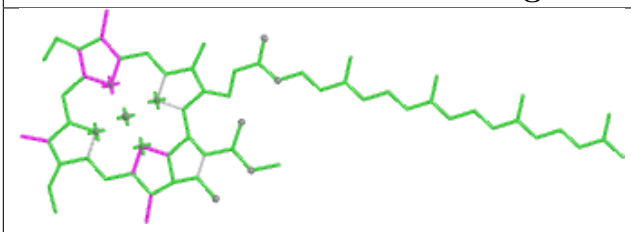


Torsions

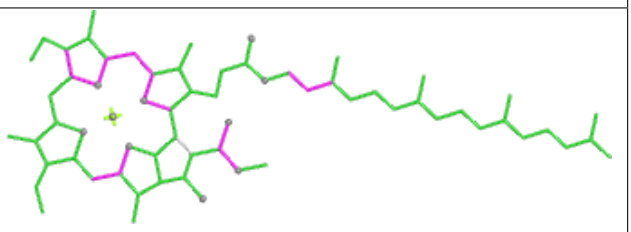


Rings

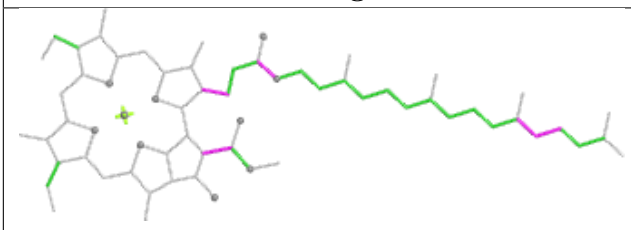
Ligand CLA A 604



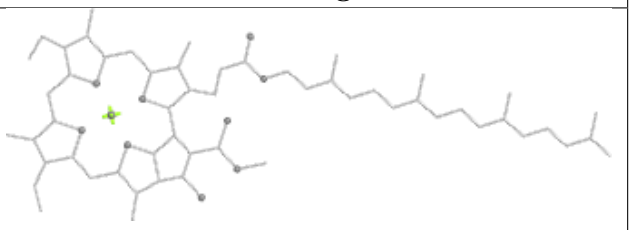
Bond lengths



Bond angles



Torsions



Rings

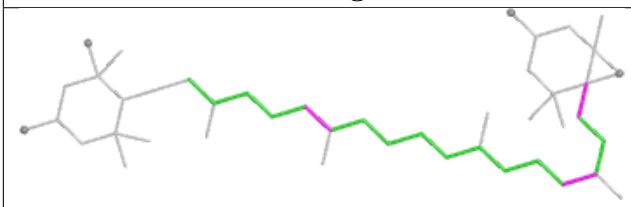
Ligand NEX N 303



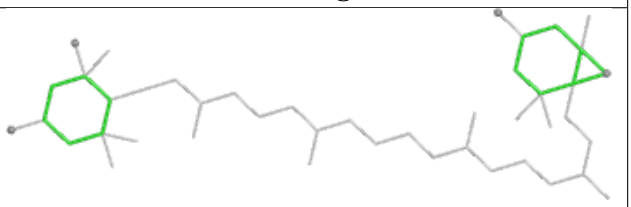
Bond lengths



Bond angles

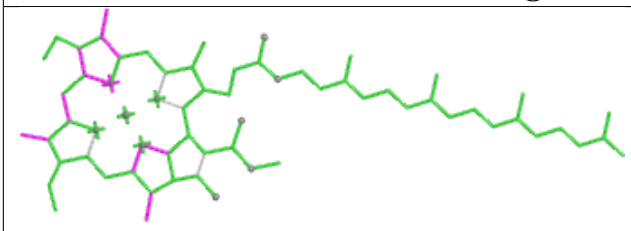


Torsions

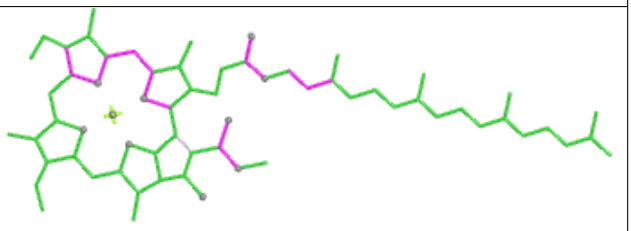


Rings

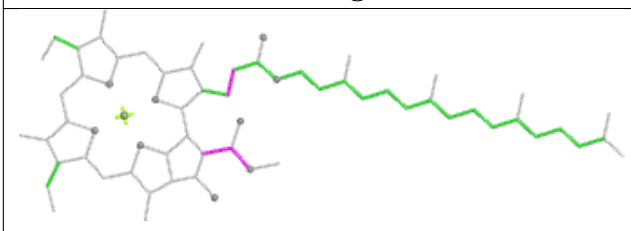
Ligand CLA B 610



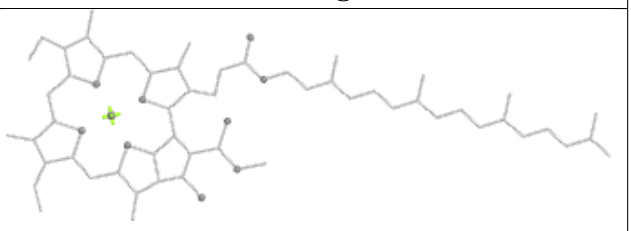
Bond lengths



Bond angles

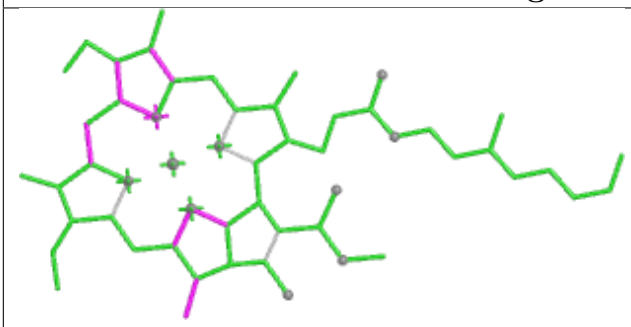


Torsions

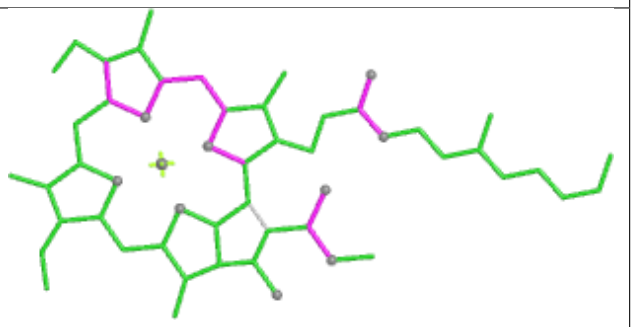


Rings

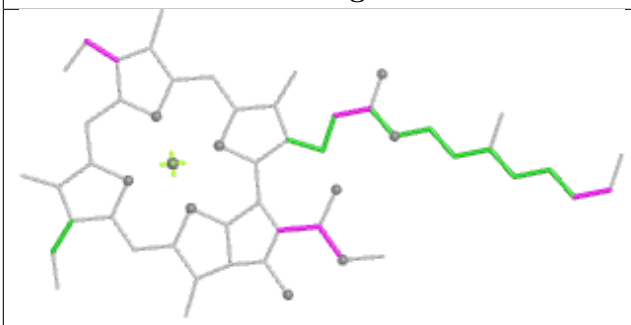
Ligand CLA n 306



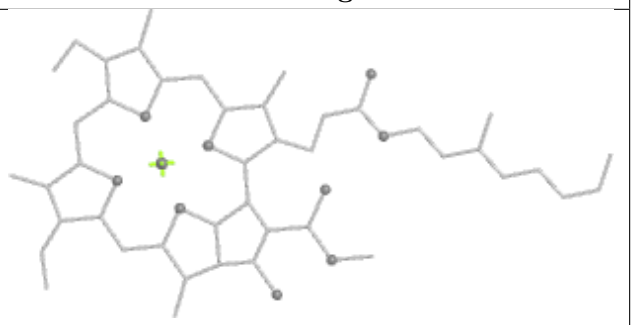
Bond lengths



Bond angles

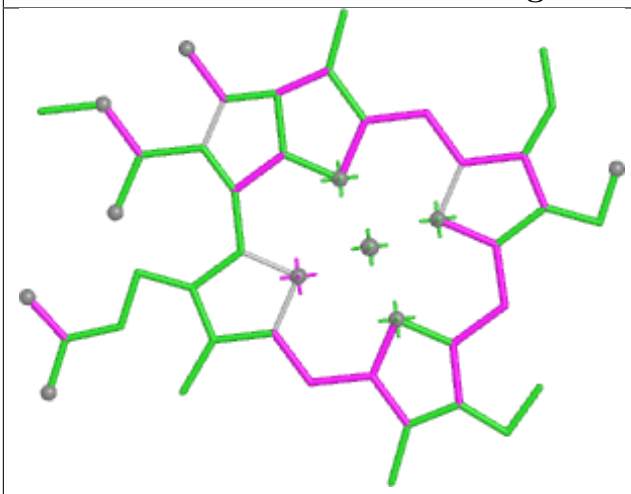


Torsions

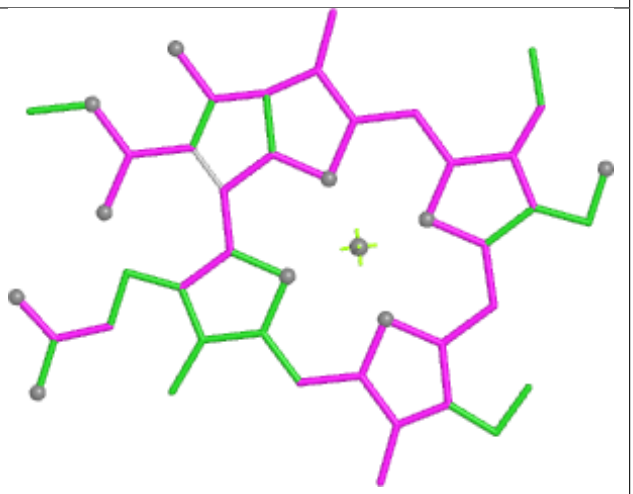


Rings

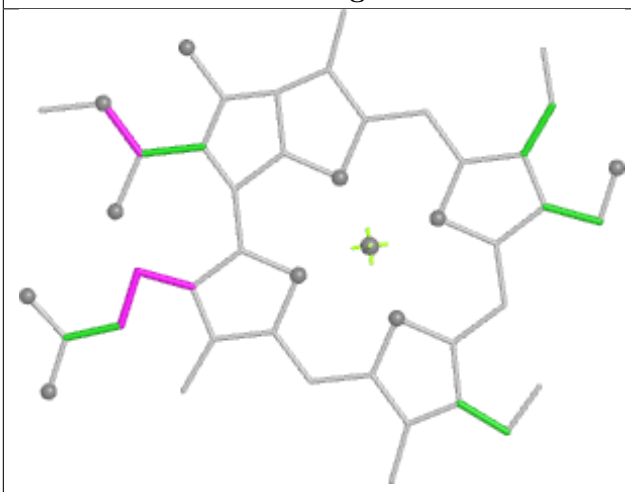
Ligand CHL S 607



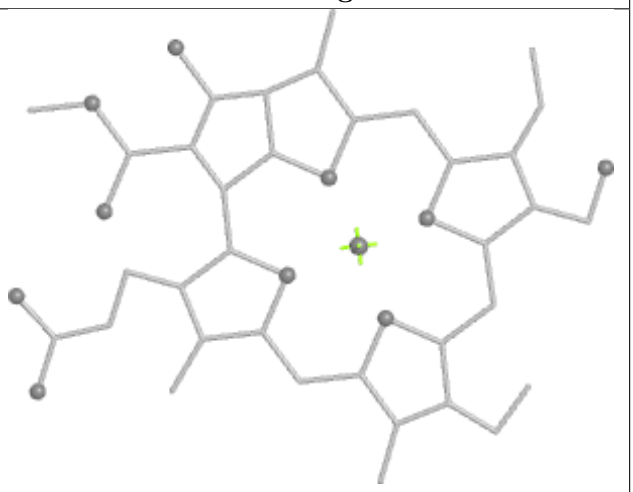
Bond lengths



Bond angles

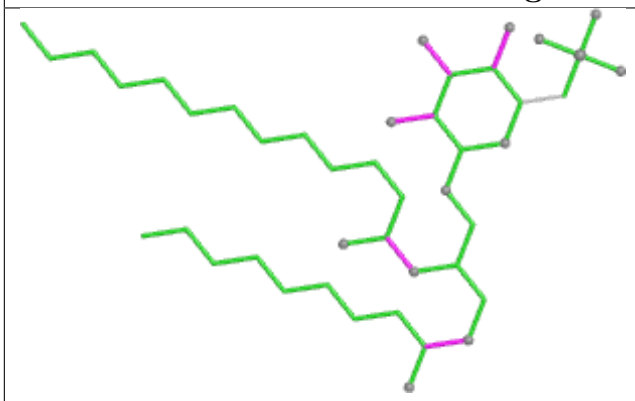


Torsions

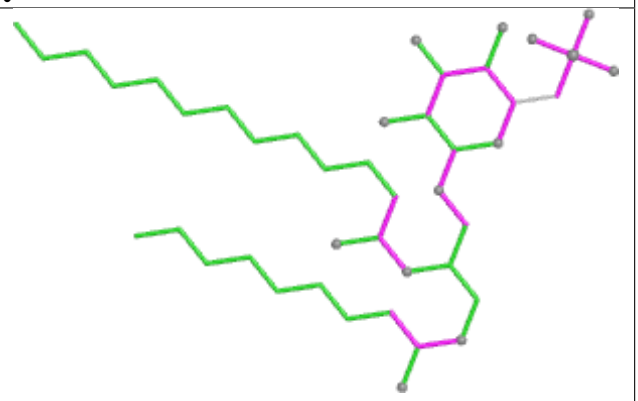


Rings

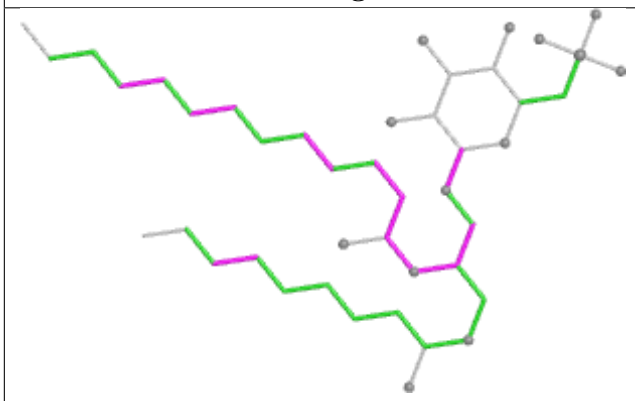
Ligand SQD D 409



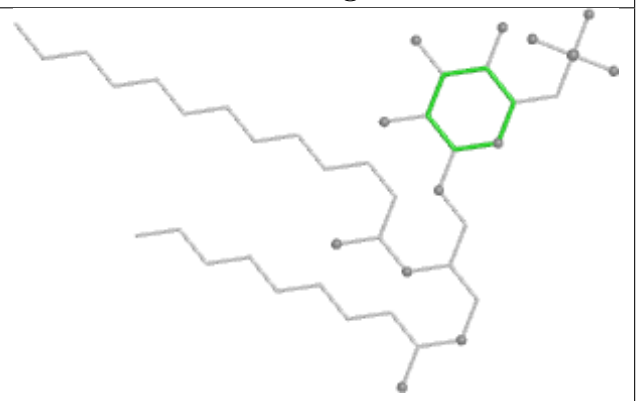
Bond lengths



Bond angles

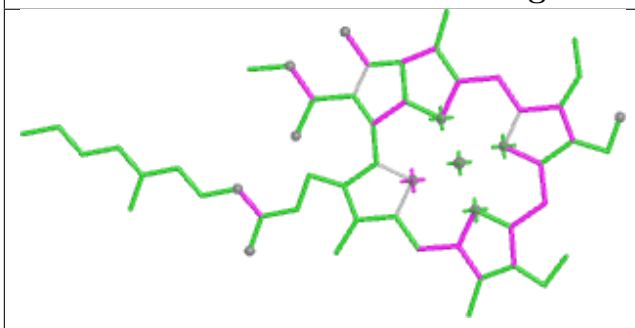


Torsions

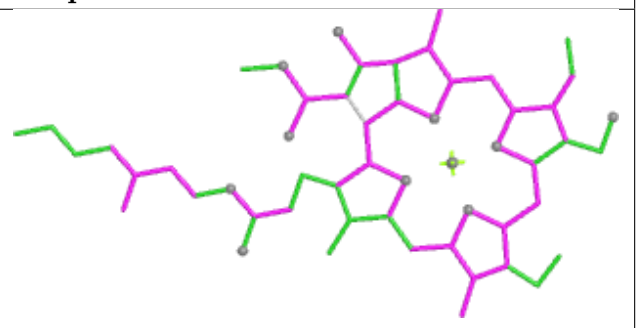


Rings

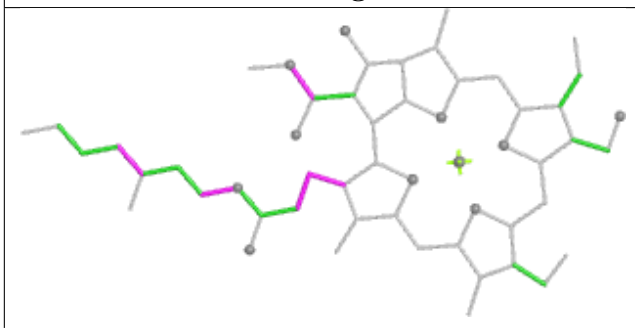
Ligand CHL q 303



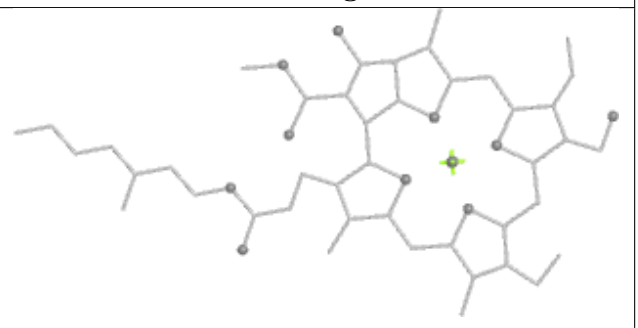
Bond lengths



Bond angles

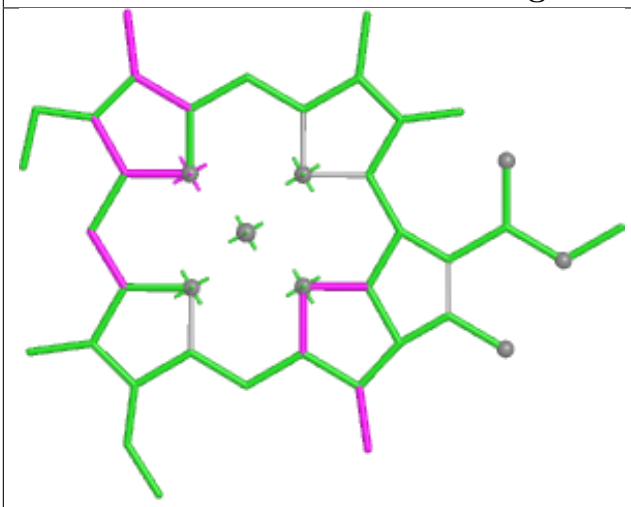


Torsions

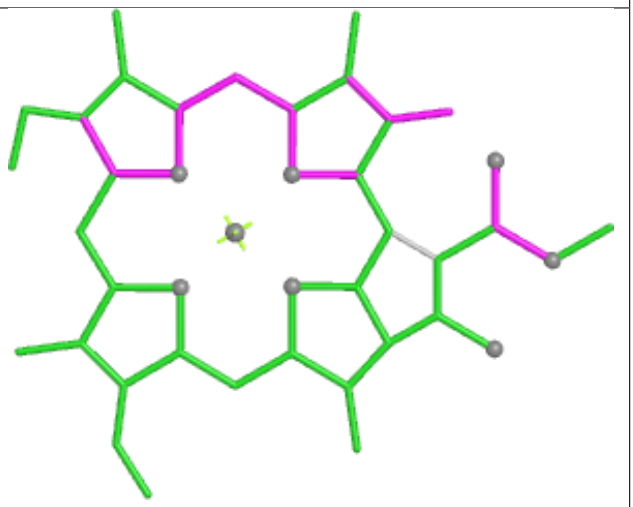


Rings

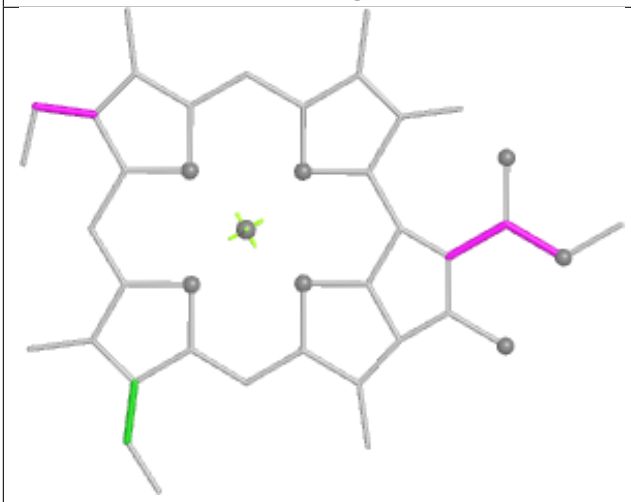
Ligand CLA 6 306



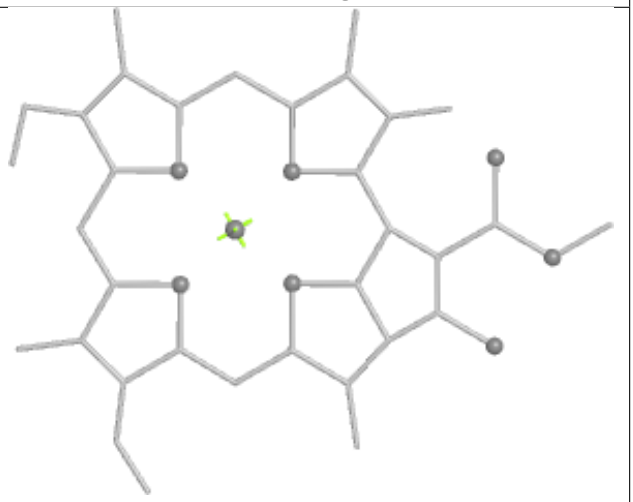
Bond lengths



Bond angles

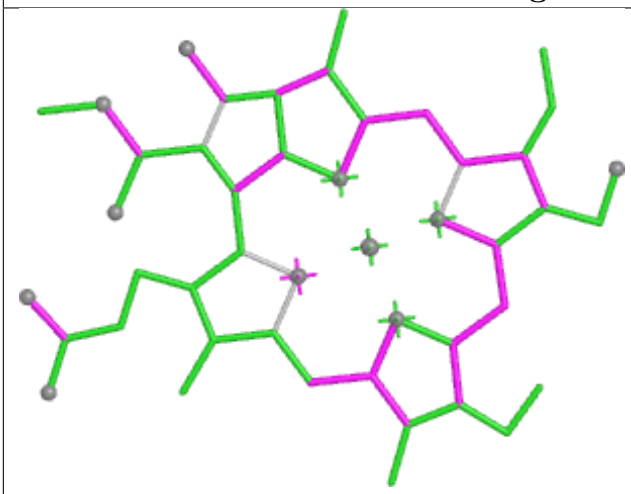


Torsions

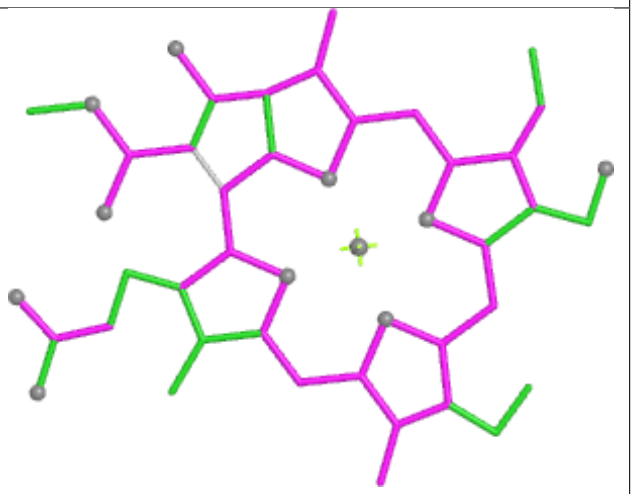


Rings

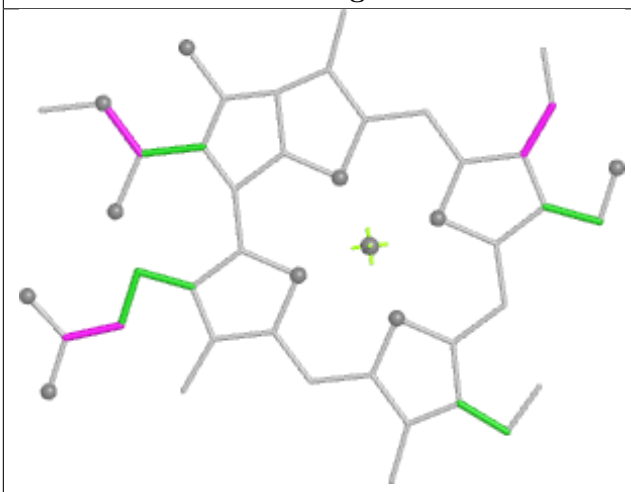
Ligand CHL r 309



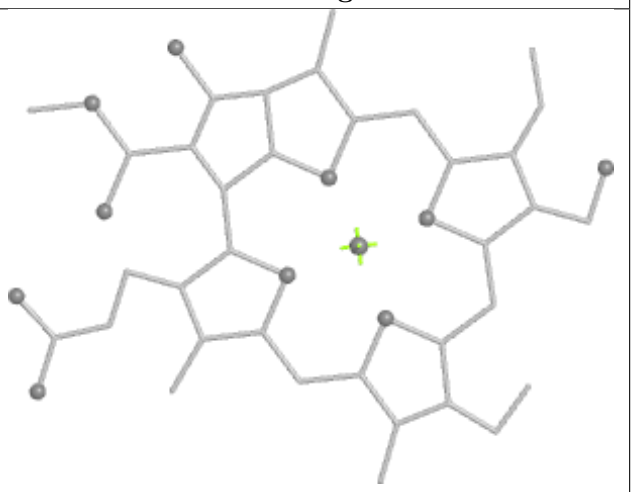
Bond lengths



Bond angles

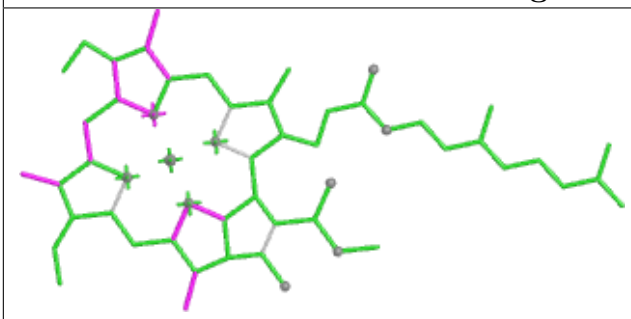


Torsions

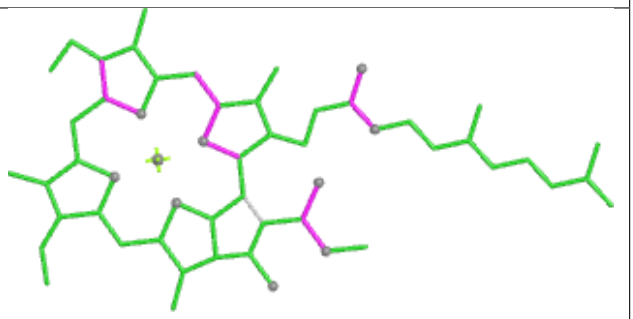


Rings

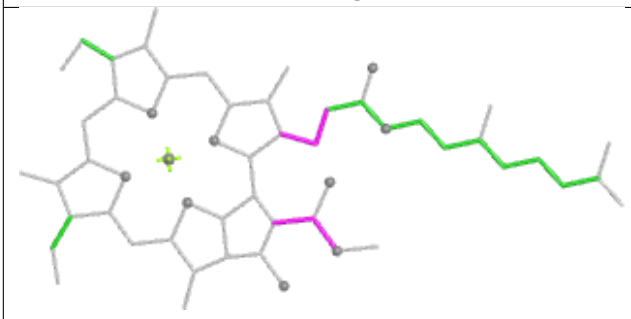
Ligand CLA s 410



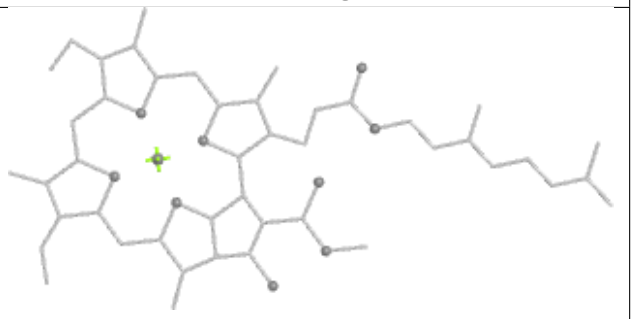
Bond lengths



Bond angles

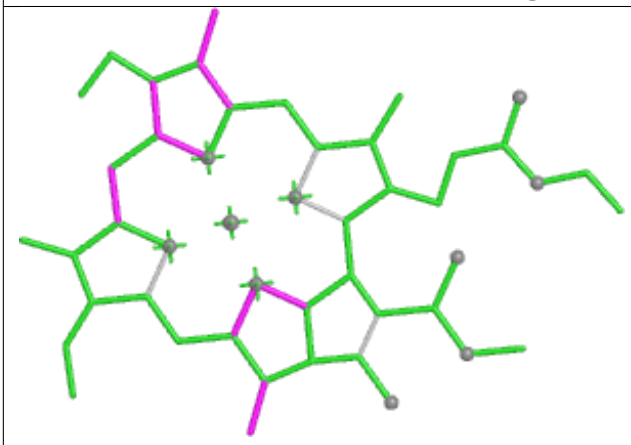


Torsions

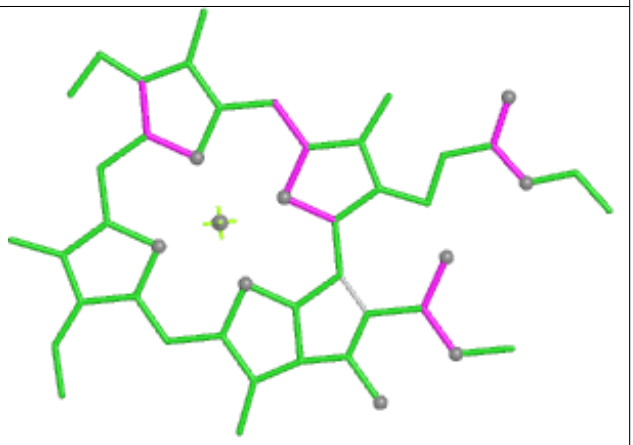


Rings

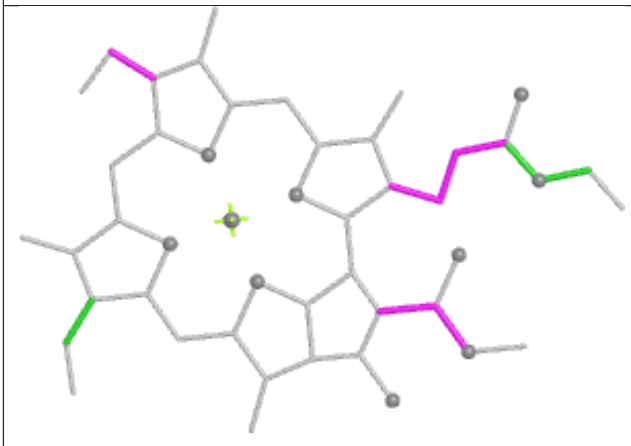
Ligand CLA R 613



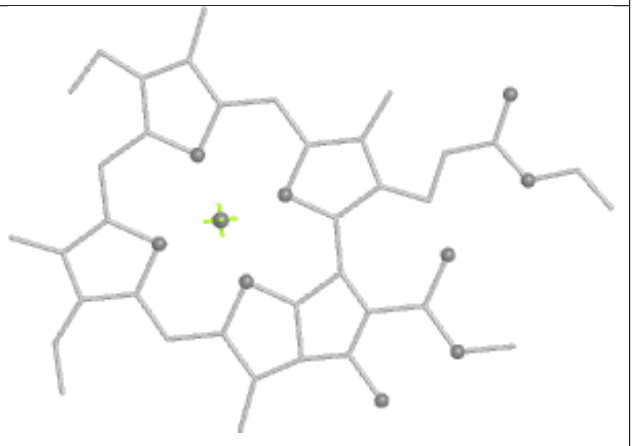
Bond lengths



Bond angles

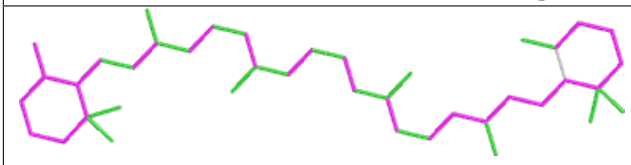


Torsions

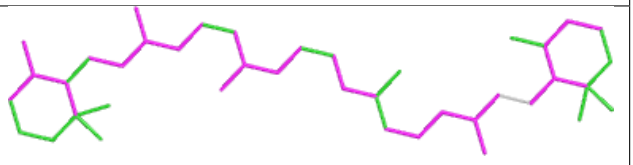


Rings

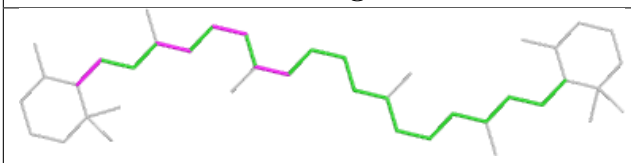
Ligand 8CT s 415



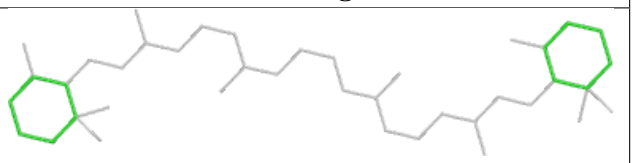
Bond lengths



Bond angles

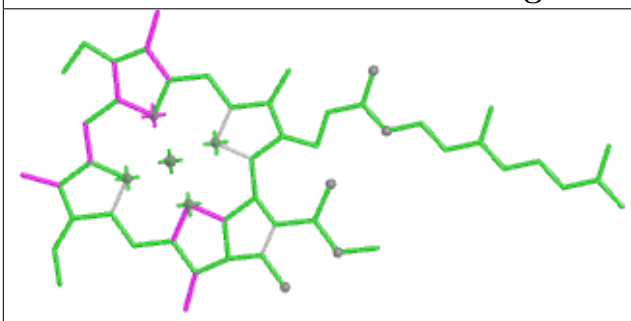


Torsions

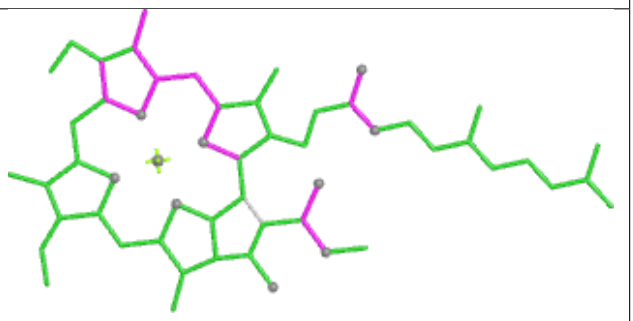


Rings

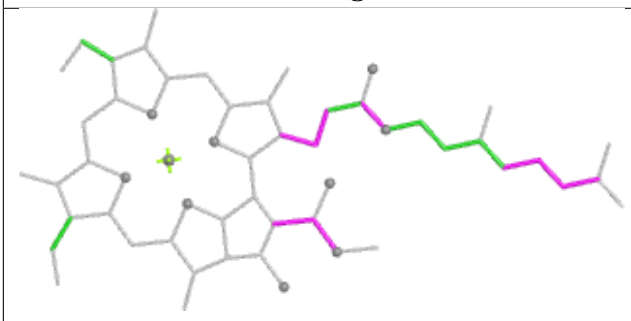
Ligand CLA B 608



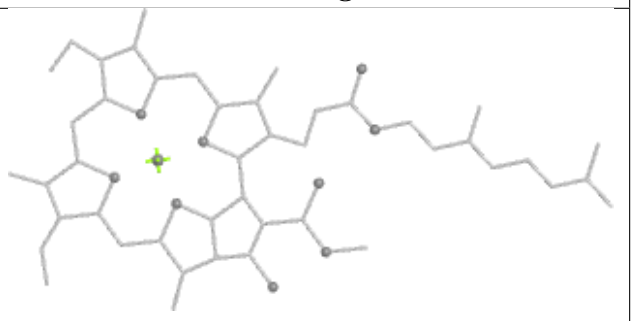
Bond lengths



Bond angles

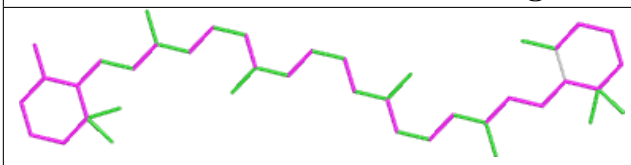


Torsions

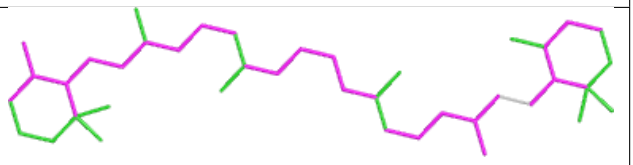


Rings

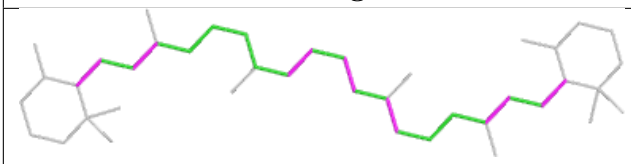
Ligand 8CT V 401



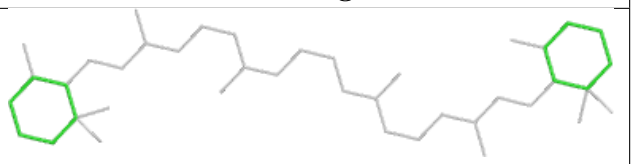
Bond lengths



Bond angles

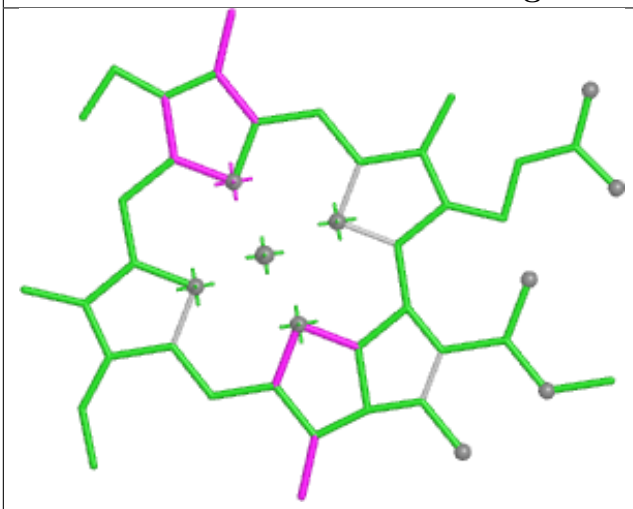


Torsions

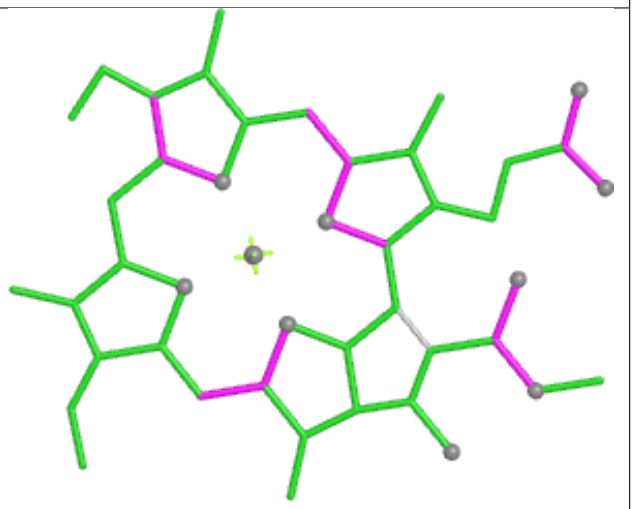


Rings

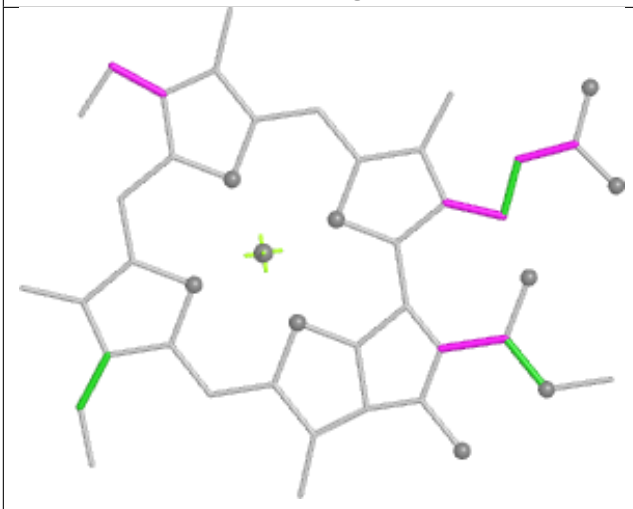
Ligand CLA R 612



Bond lengths



Bond angles

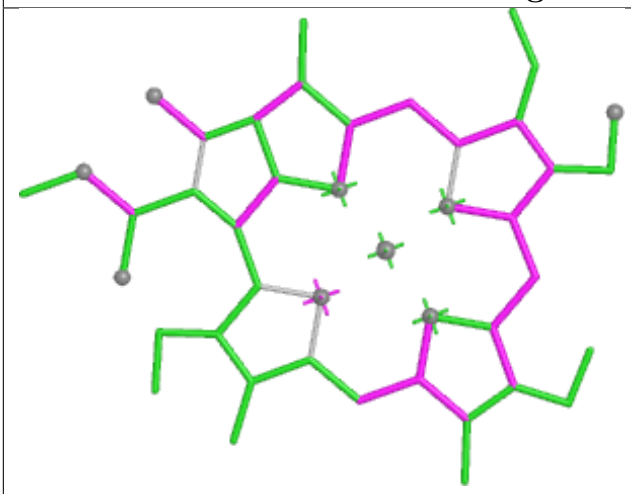


Torsions

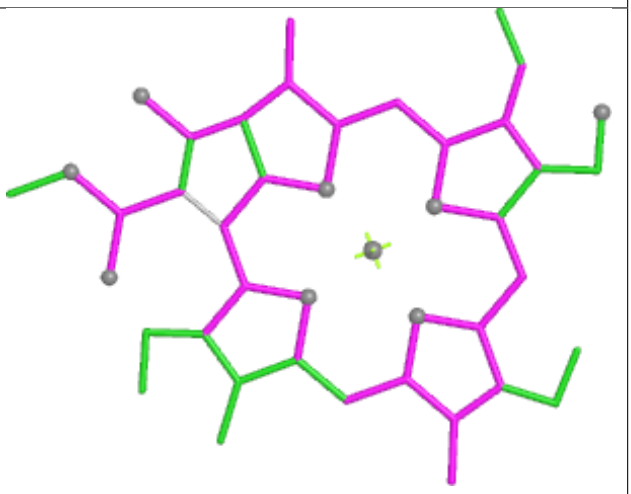


Rings

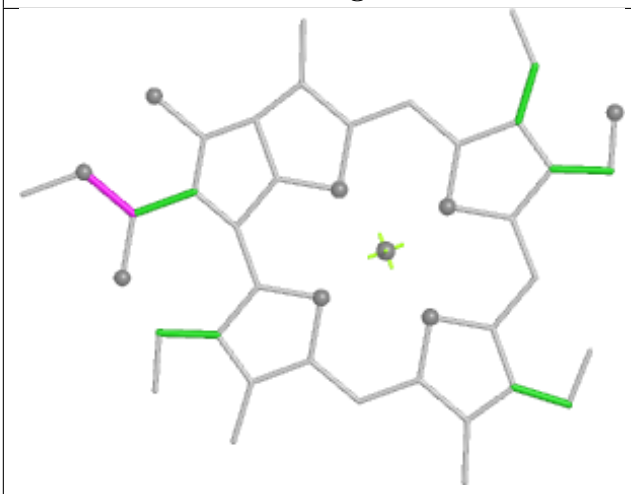
Ligand CHL u 309



Bond lengths



Bond angles



Torsions



Rings

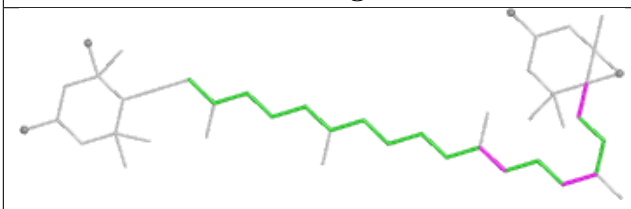
Ligand NEX p 304



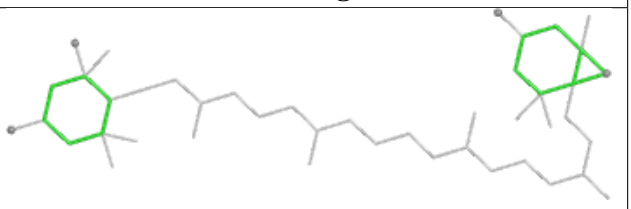
Bond lengths



Bond angles

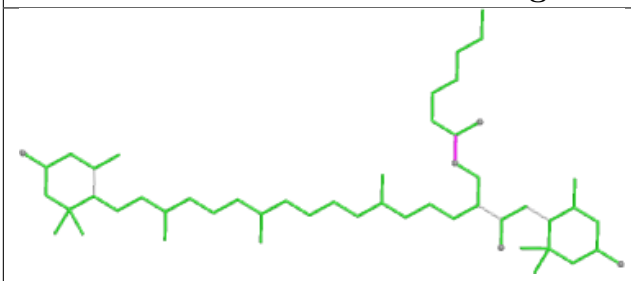


Torsions

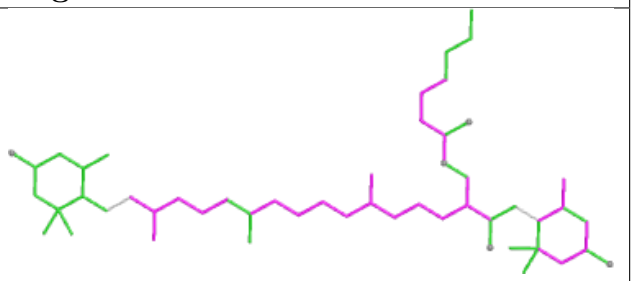


Rings

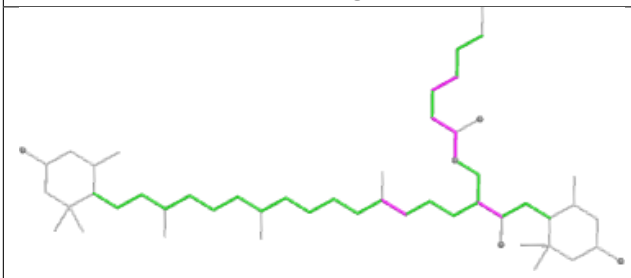
Ligand 0UR g 301



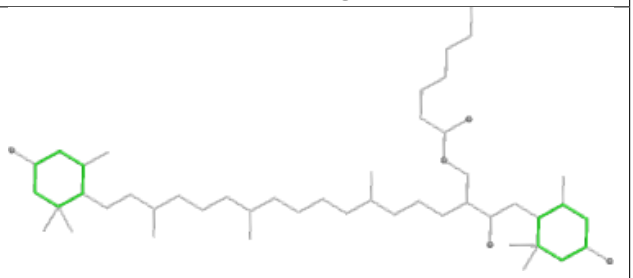
Bond lengths



Bond angles

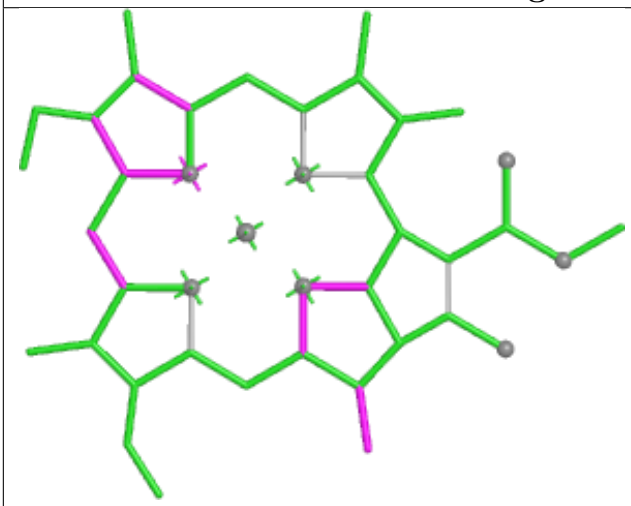


Torsions

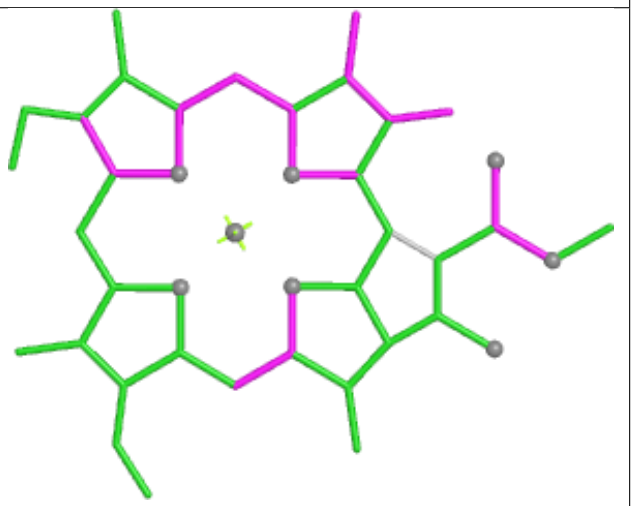


Rings

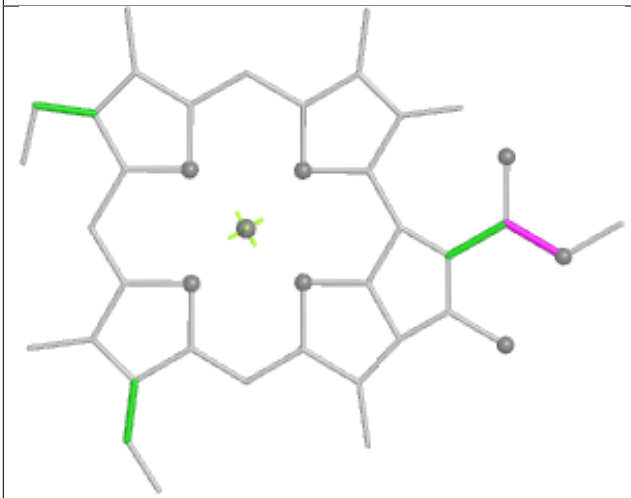
Ligand CLA 3 313



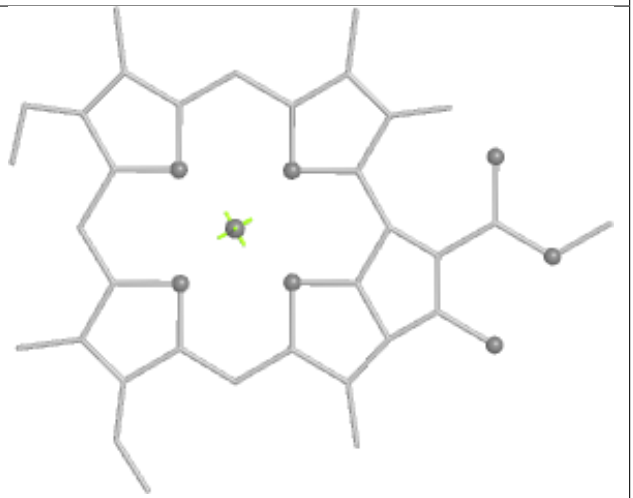
Bond lengths



Bond angles

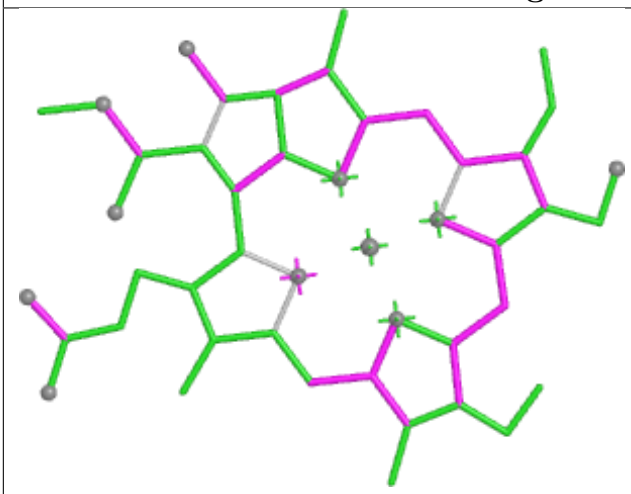


Torsions

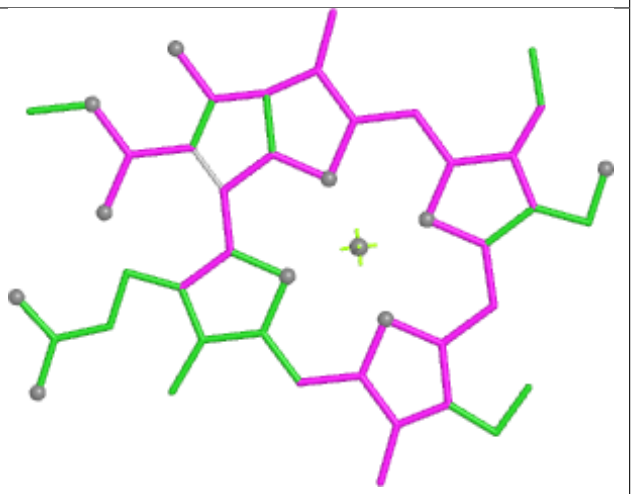


Rings

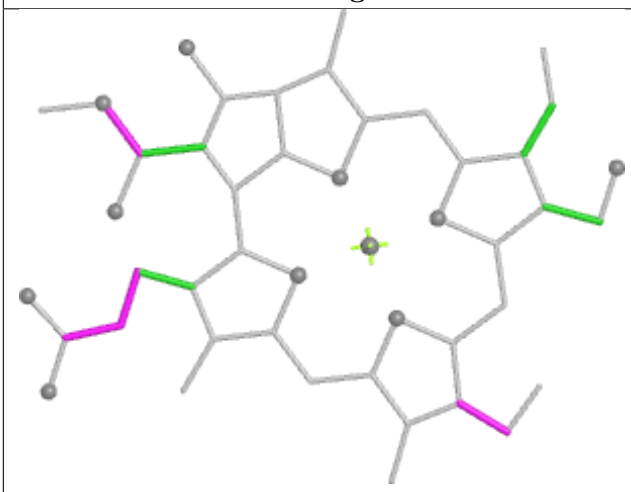
Ligand CHL S 605



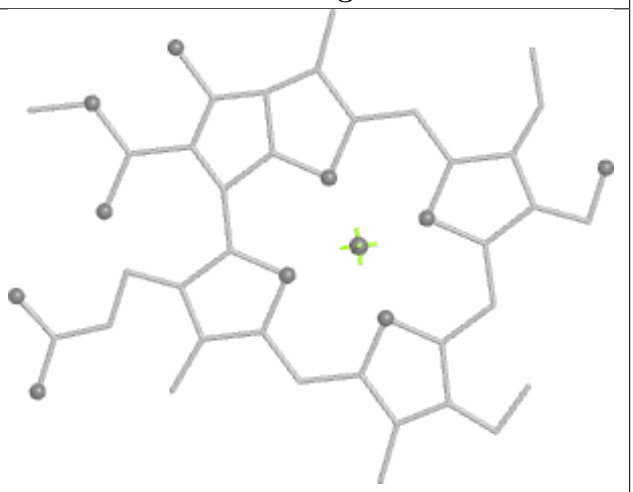
Bond lengths



Bond angles

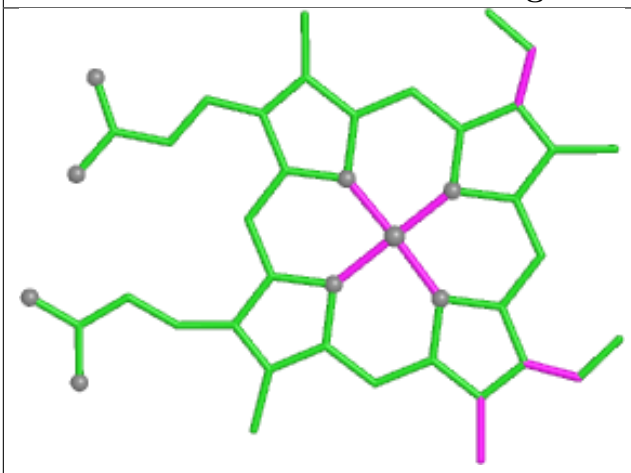


Torsions

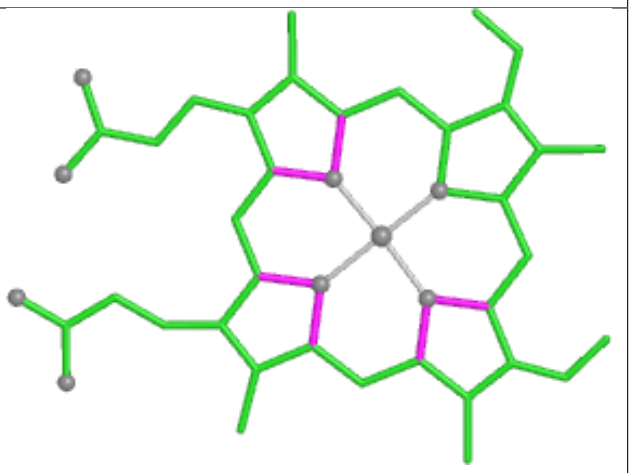


Rings

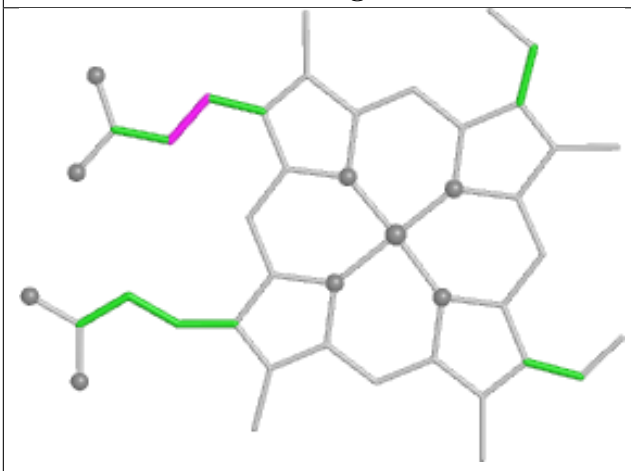
Ligand HEM f 201



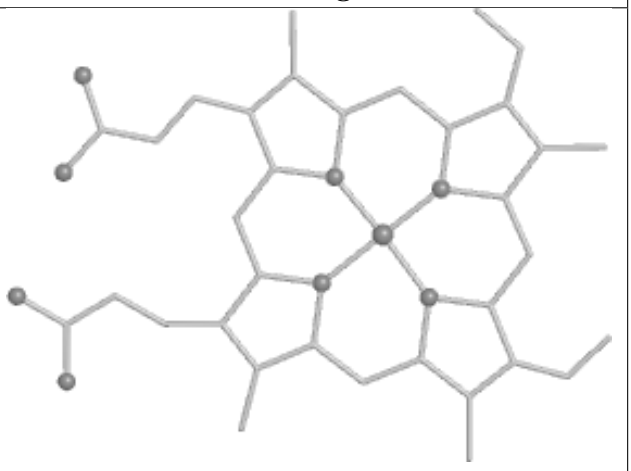
Bond lengths



Bond angles

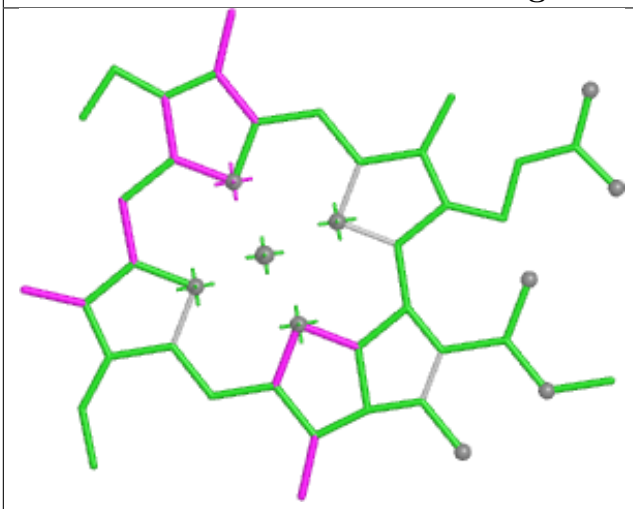


Torsions

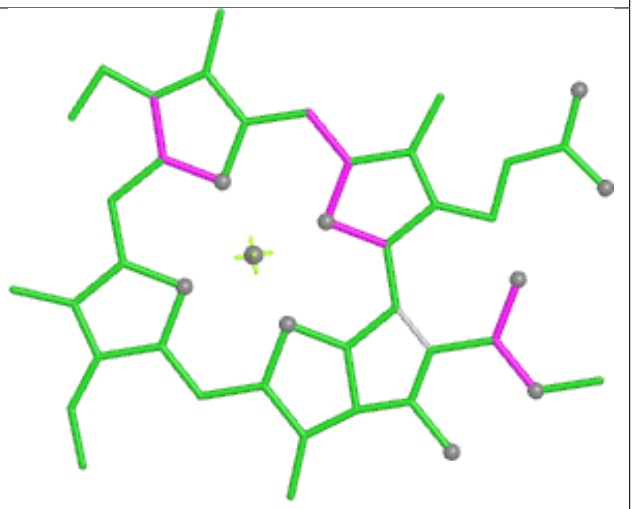


Rings

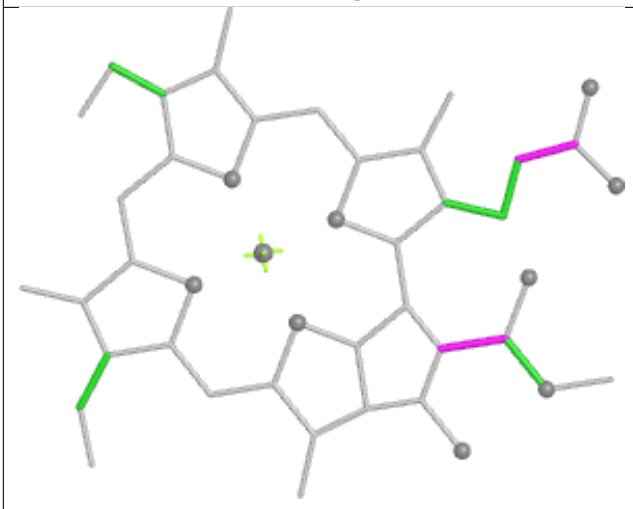
Ligand CLA 2 316



Bond lengths



Bond angles

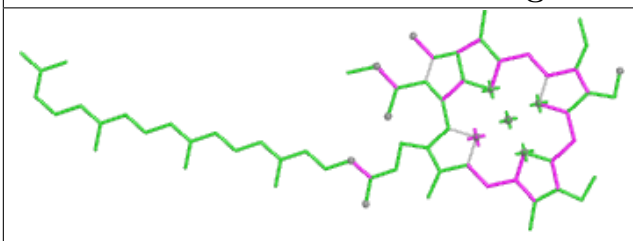


Torsions

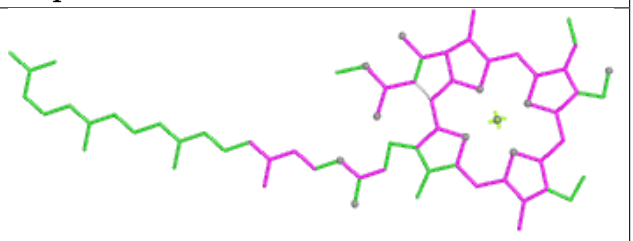


Rings

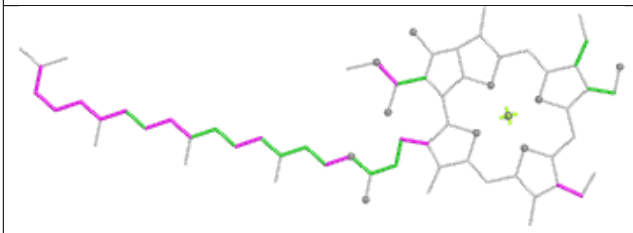
Ligand CHL p 305



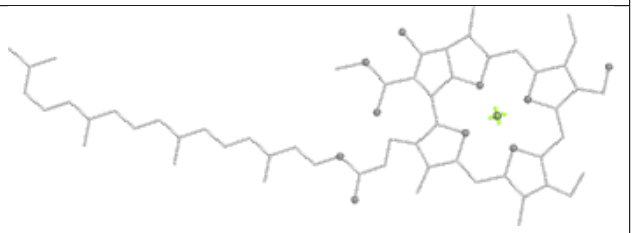
Bond lengths



Bond angles

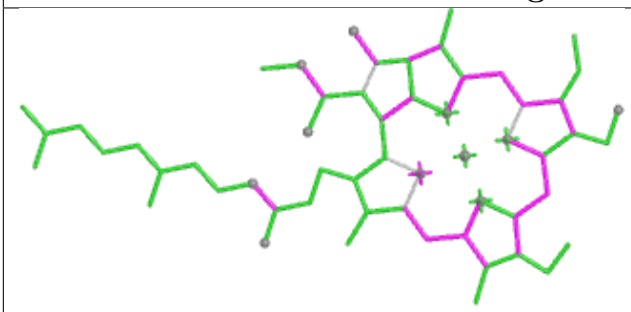


Torsions

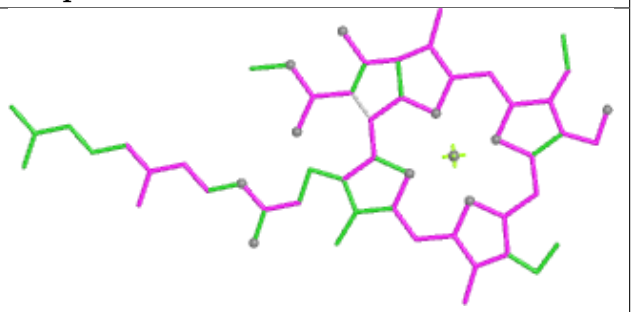


Rings

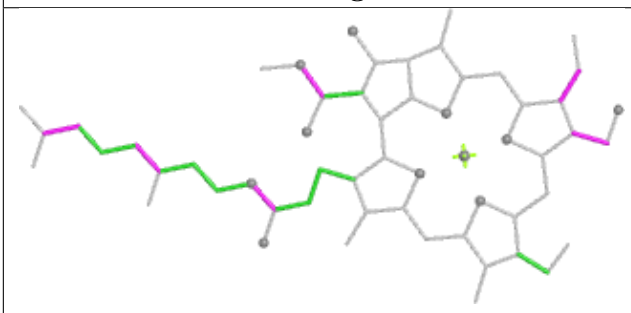
Ligand CHL q 311



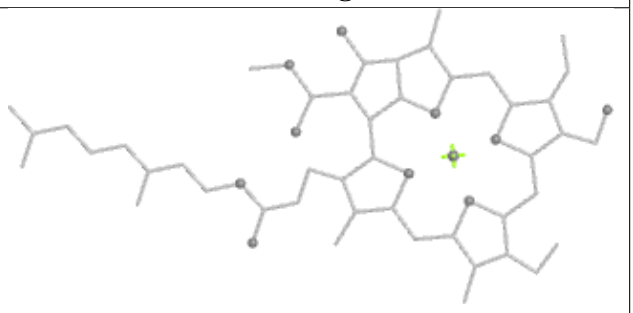
Bond lengths



Bond angles

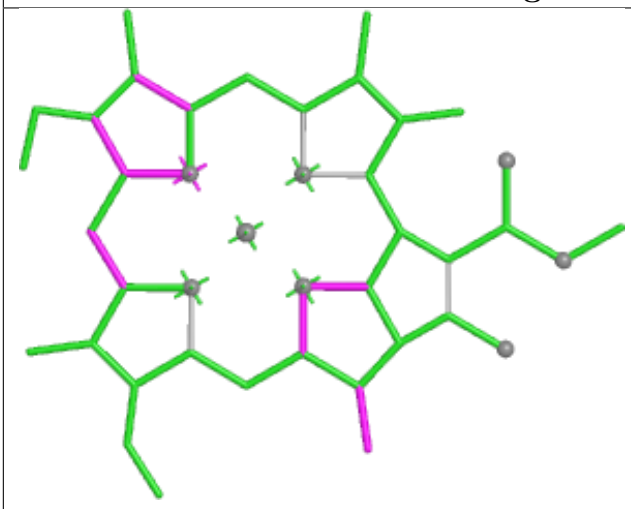


Torsions

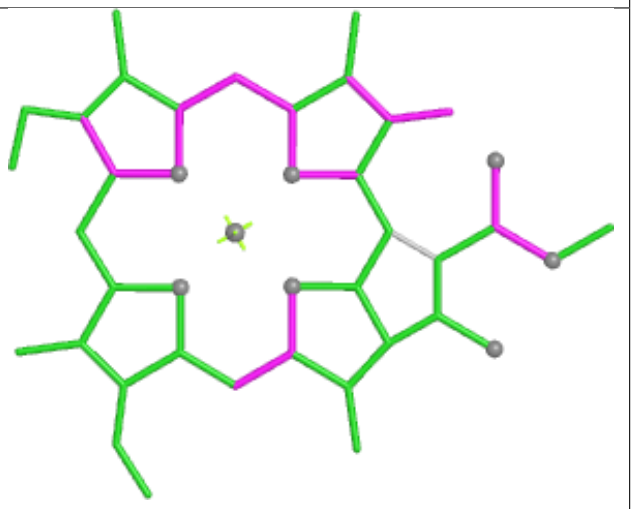


Rings

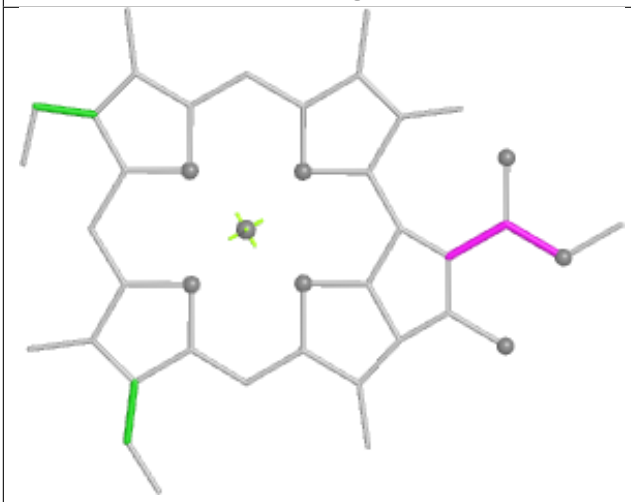
Ligand CLA A 610



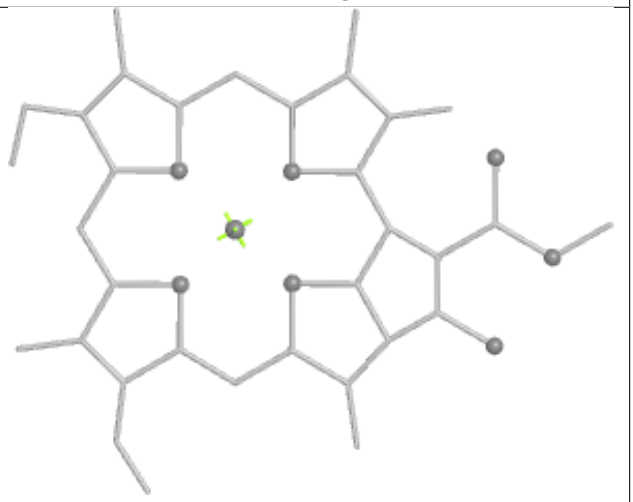
Bond lengths



Bond angles

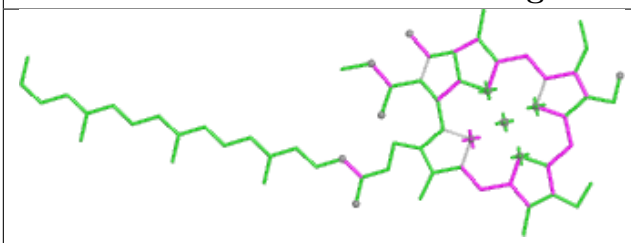


Torsions

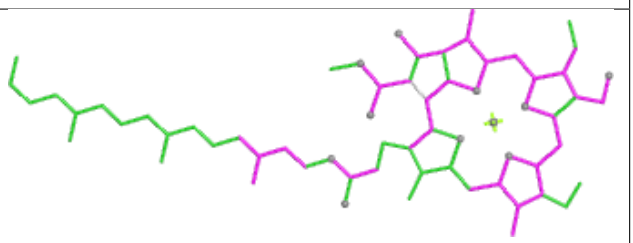


Rings

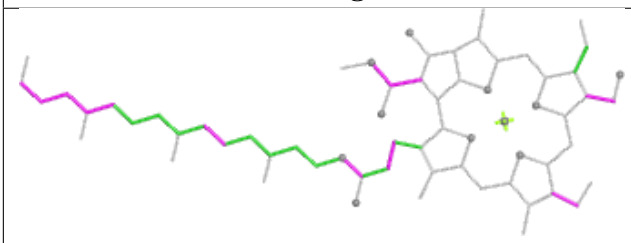
Ligand CHL u 306



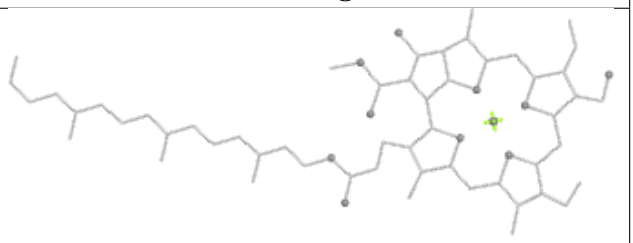
Bond lengths



Bond angles

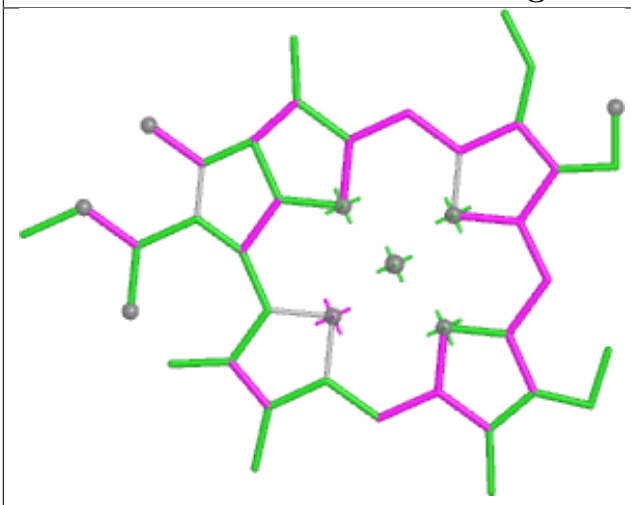


Torsions

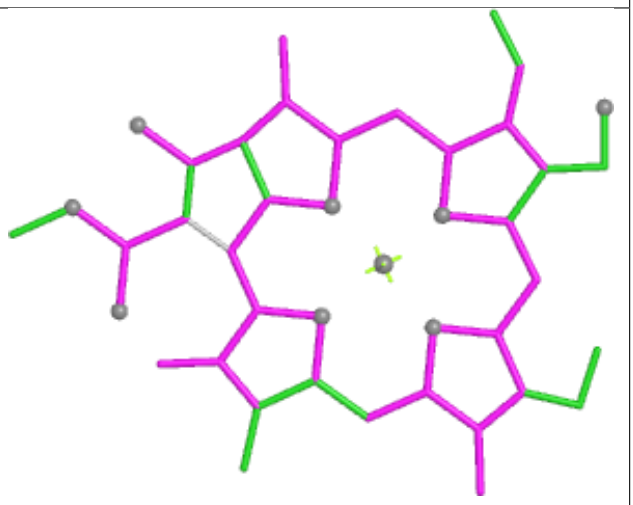


Rings

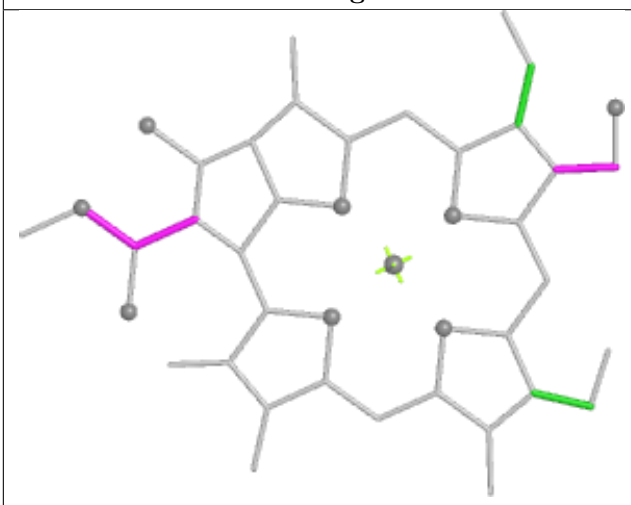
Ligand CHL 1 317



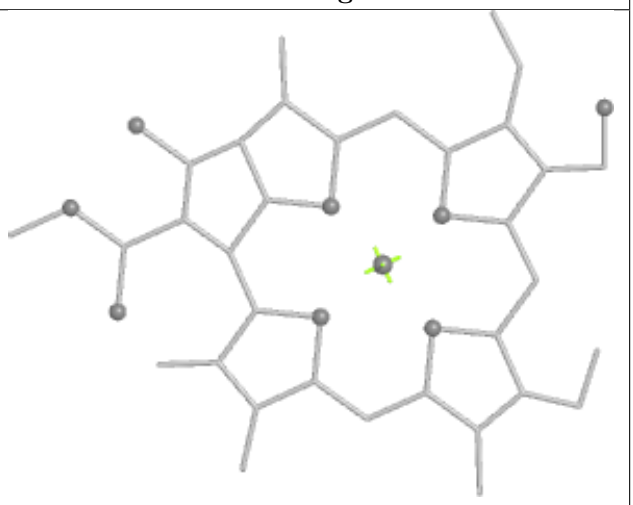
Bond lengths



Bond angles

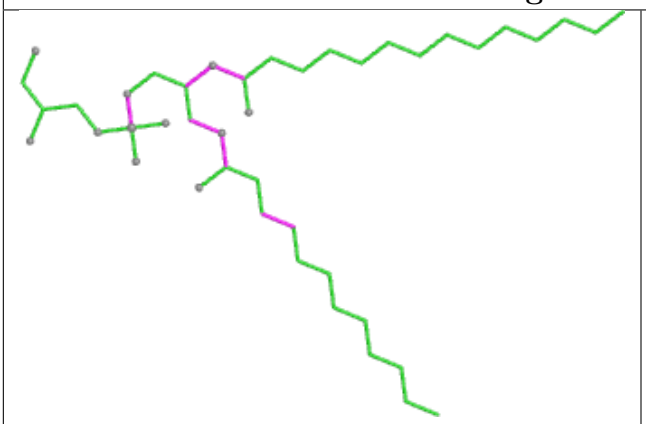


Torsions

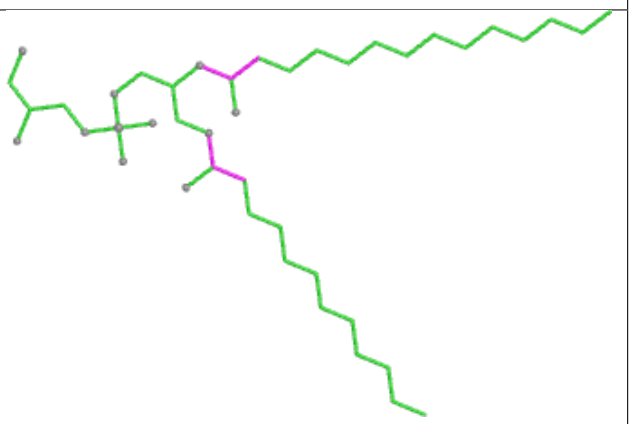


Rings

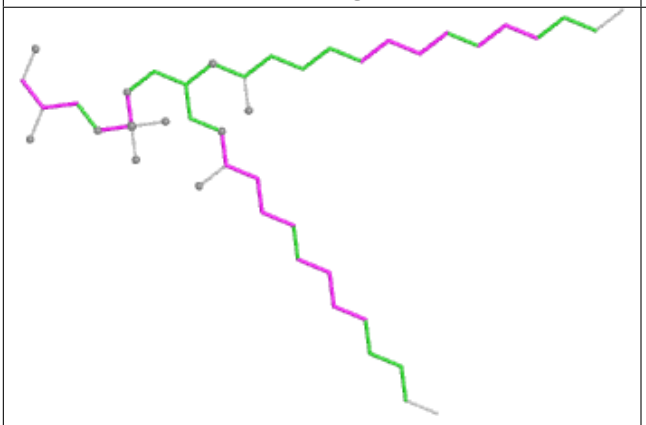
Ligand LHG n 318



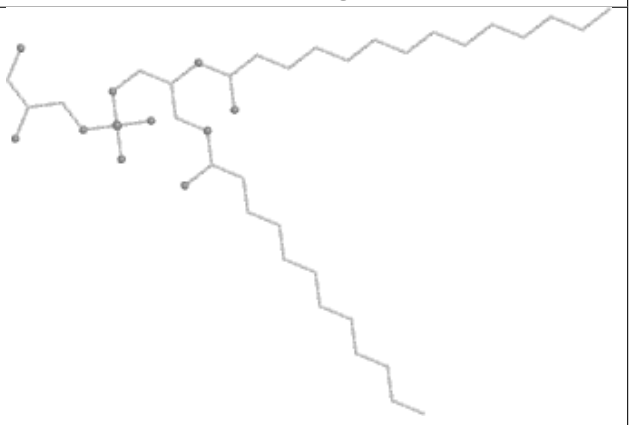
Bond lengths



Bond angles

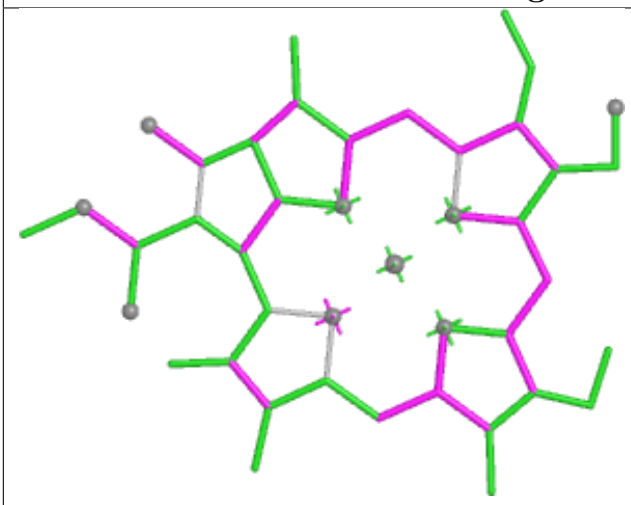


Torsions

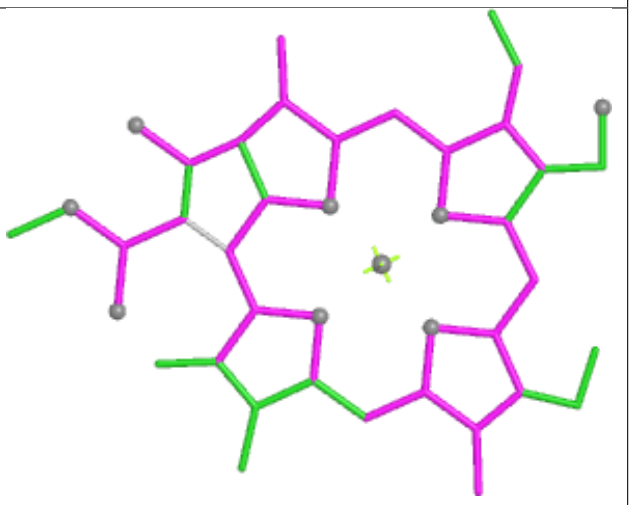


Rings

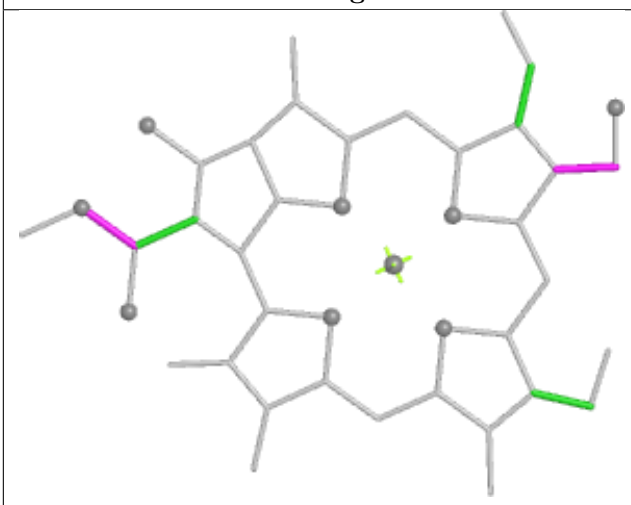
Ligand CHL 2 313



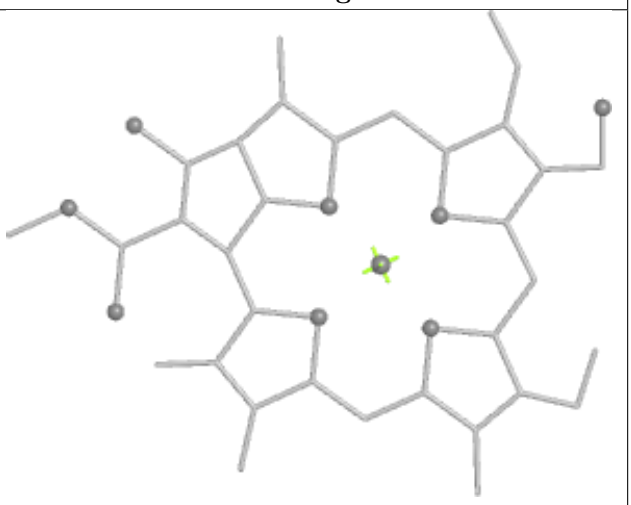
Bond lengths



Bond angles

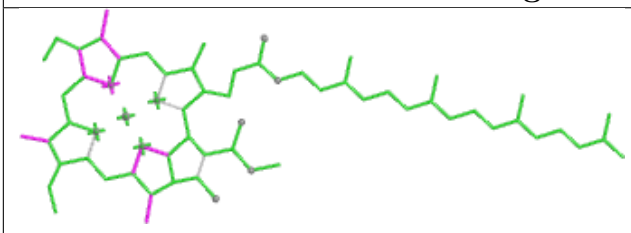


Torsions

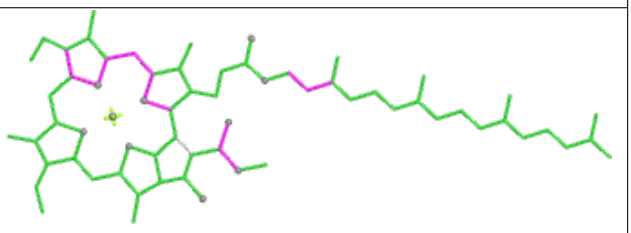


Rings

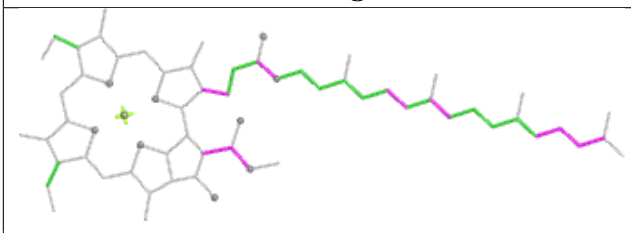
Ligand CLA D 405



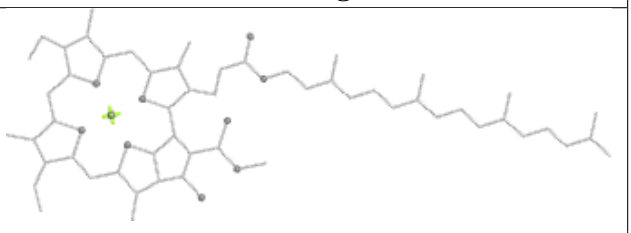
Bond lengths



Bond angles

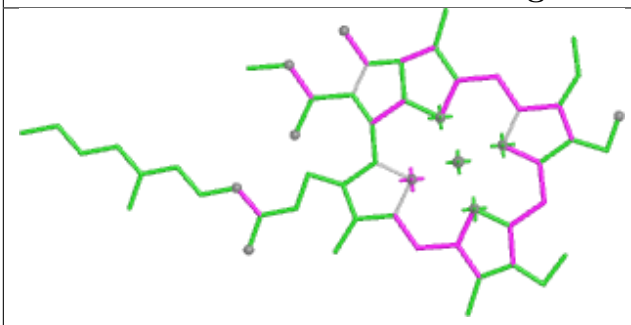


Torsions

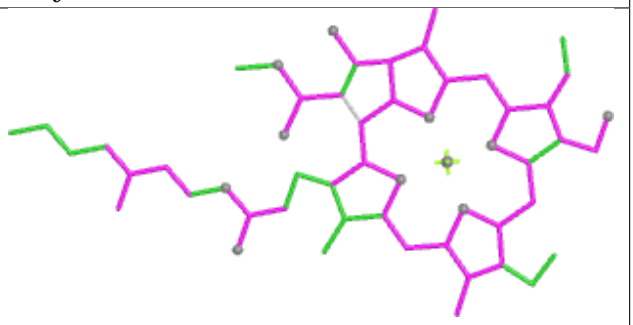


Rings

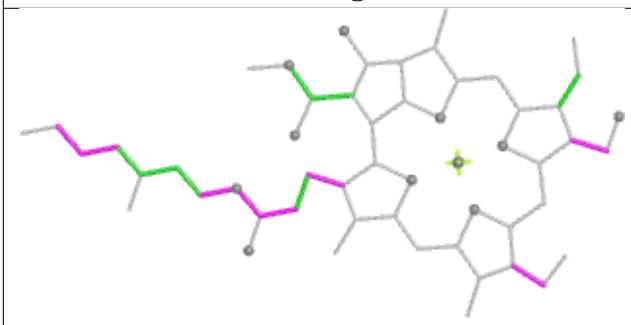
Ligand CHL y 311



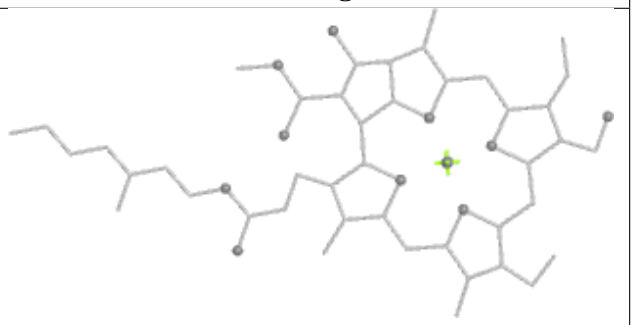
Bond lengths



Bond angles

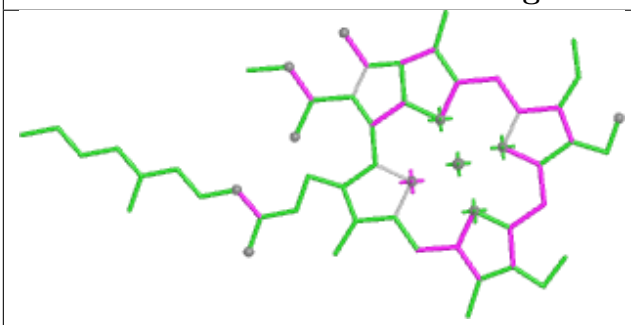


Torsions

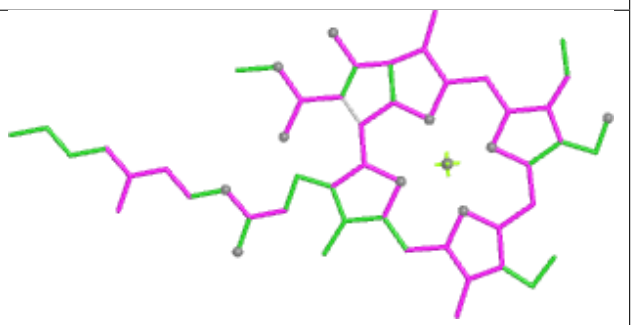


Rings

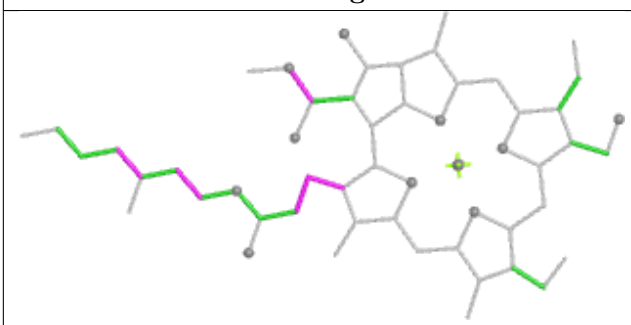
Ligand CHL N 304



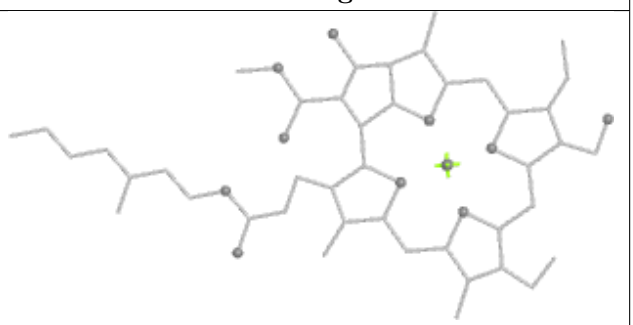
Bond lengths



Bond angles

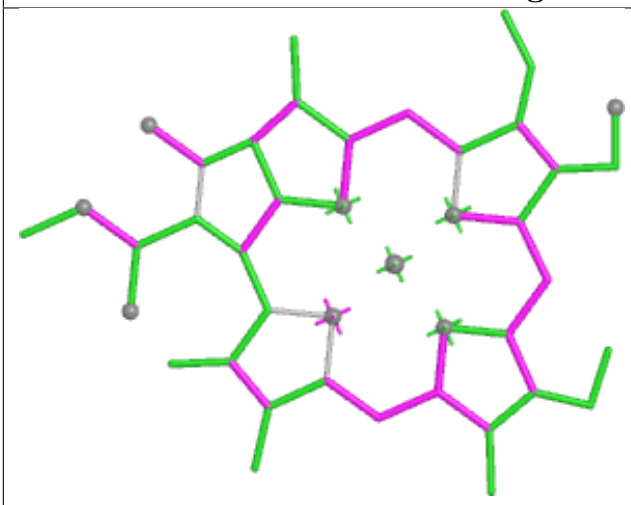


Torsions

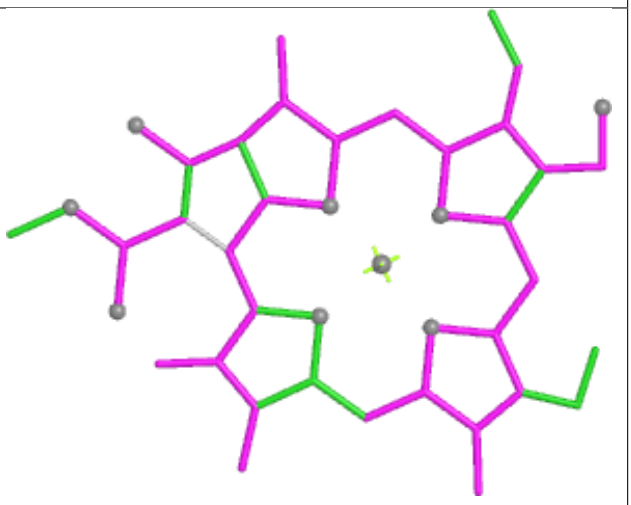


Rings

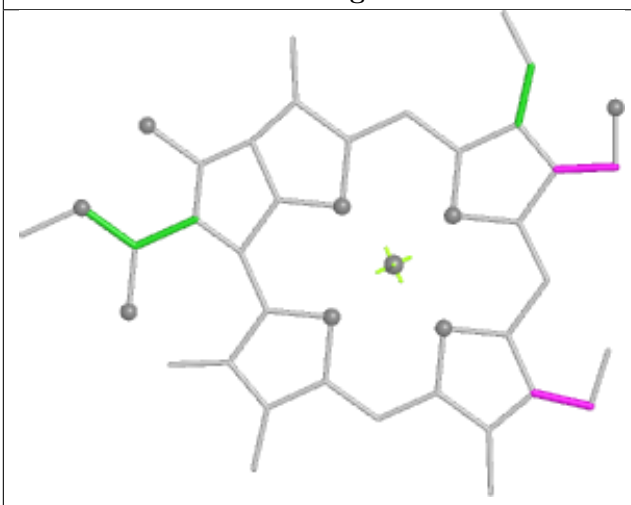
Ligand CHL S 613



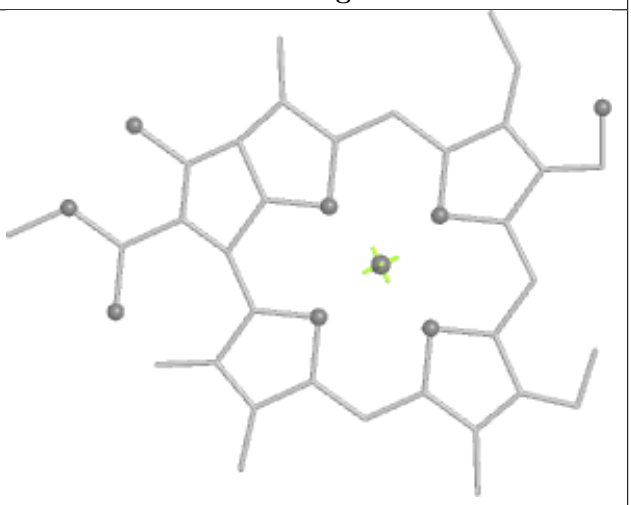
Bond lengths



Bond angles

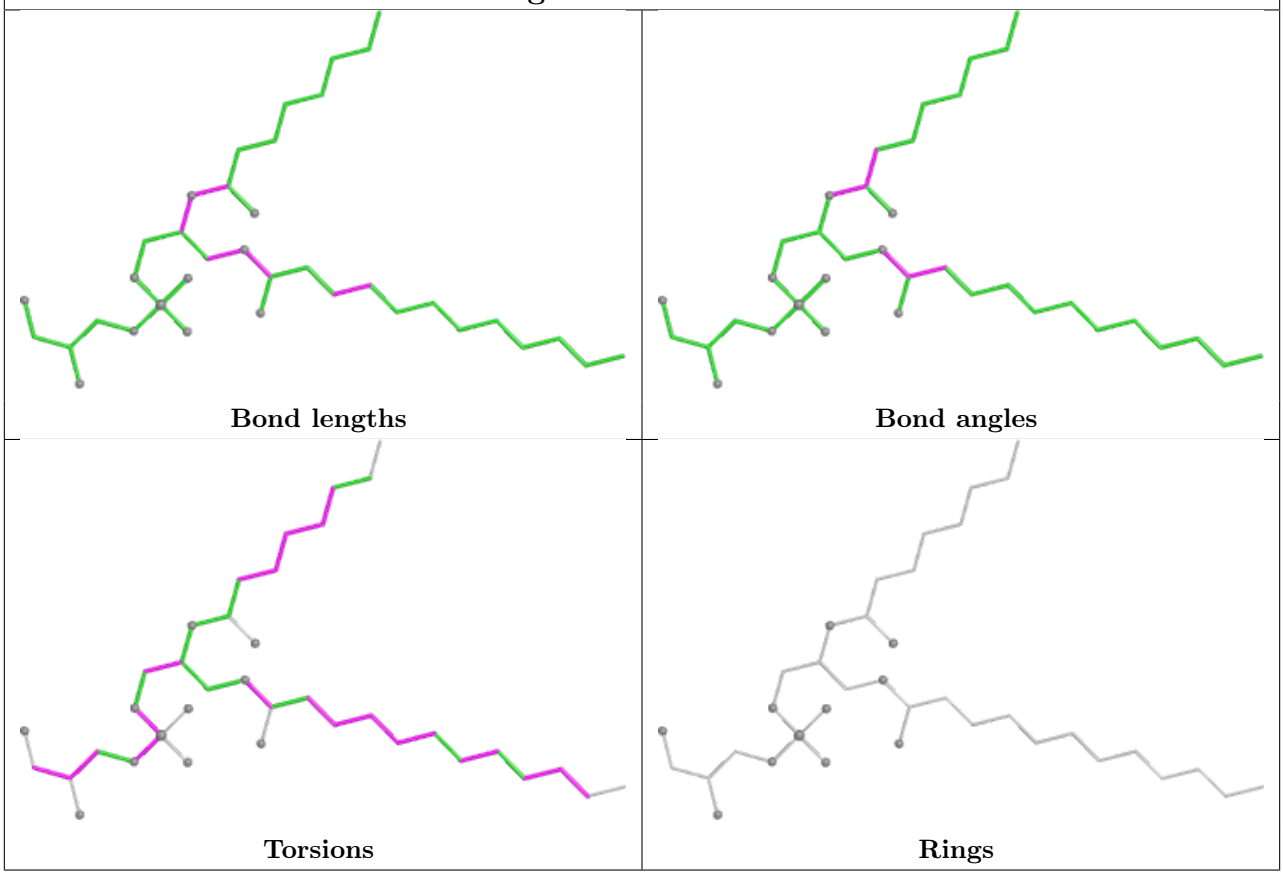


Torsions

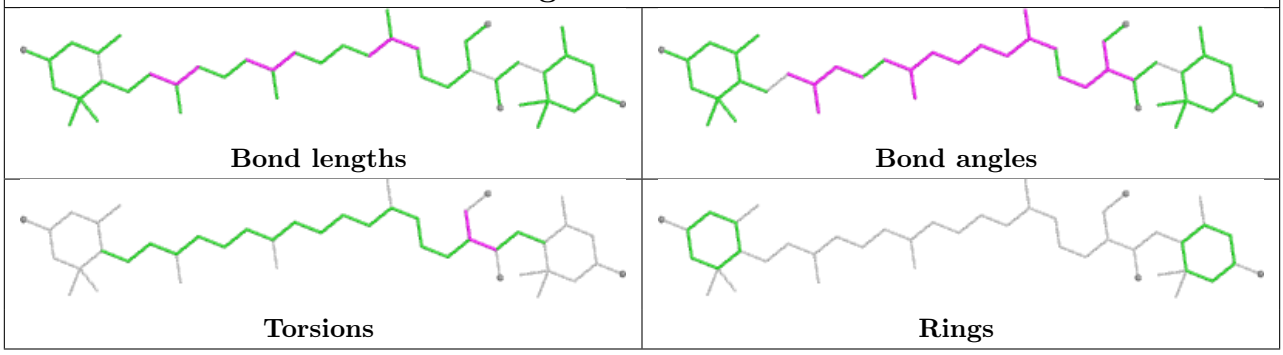


Rings

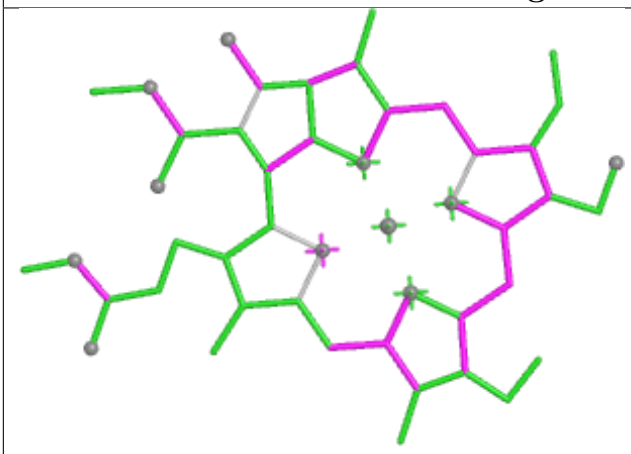
Ligand LHG 7 319



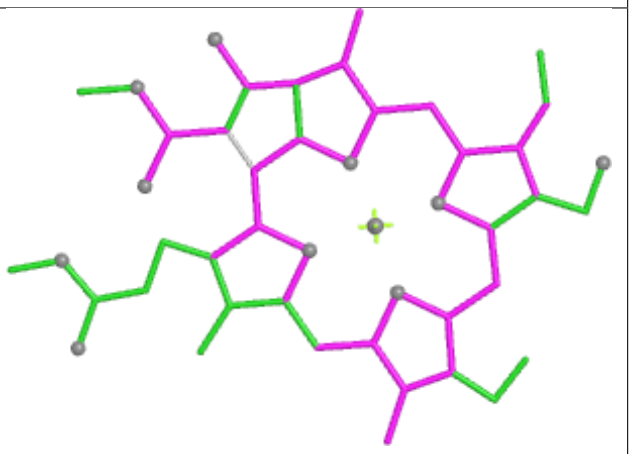
Ligand 0IE 7 302



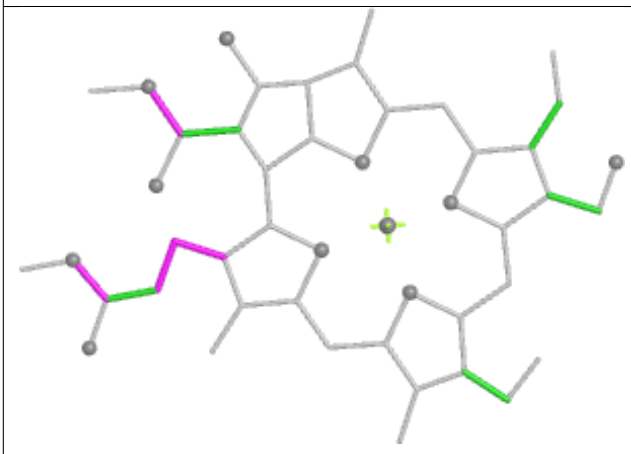
Ligand CHL 9 311



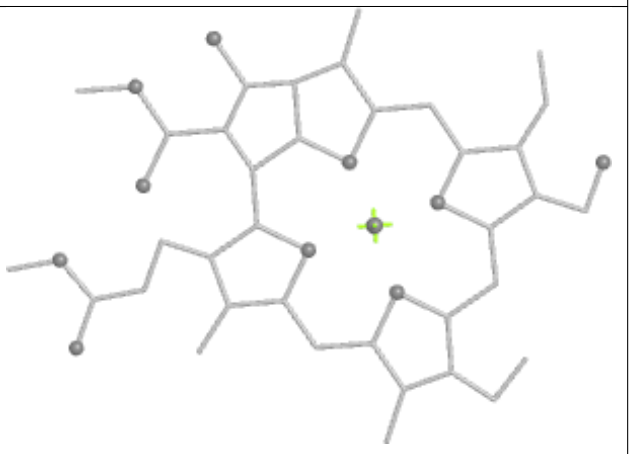
Bond lengths



Bond angles

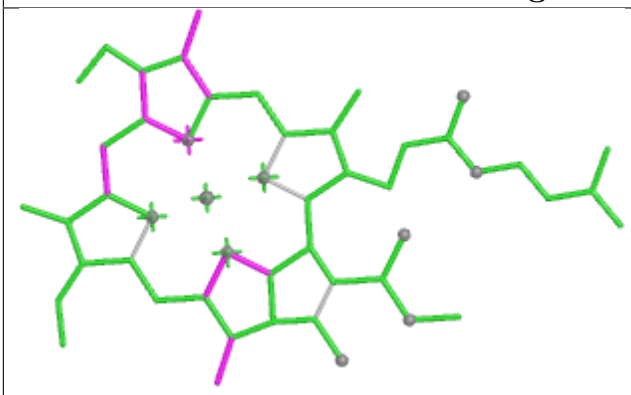


Torsions

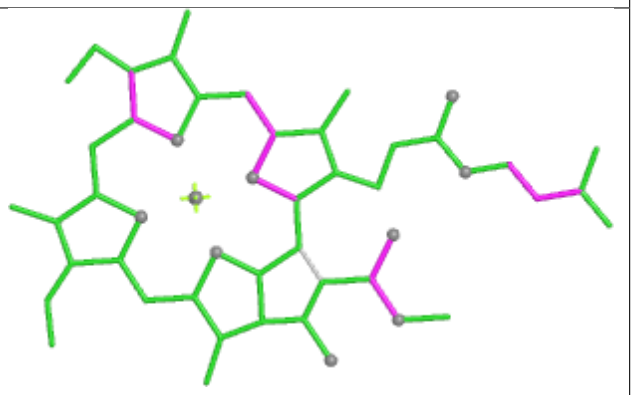


Rings

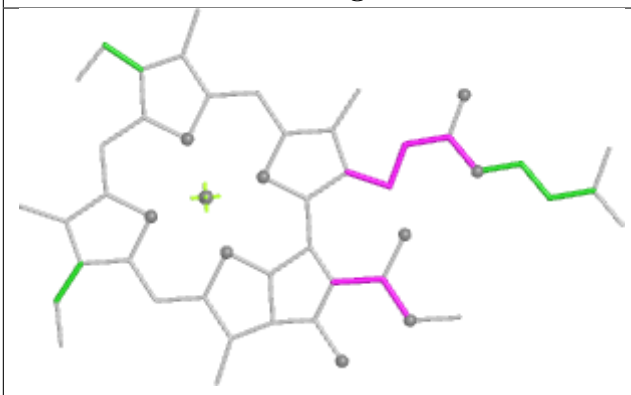
Ligand CLA 9 307



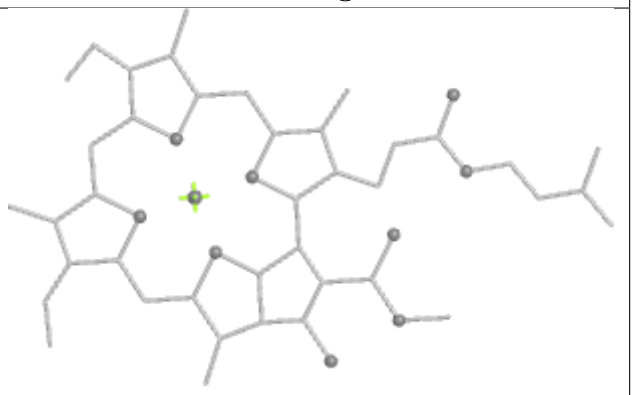
Bond lengths



Bond angles

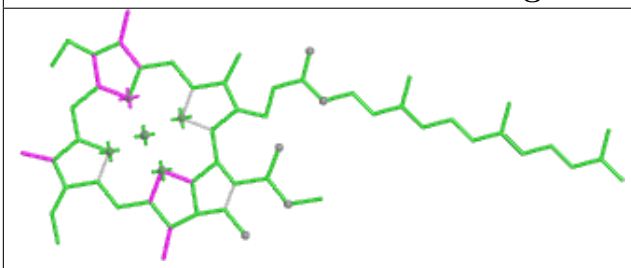


Torsions

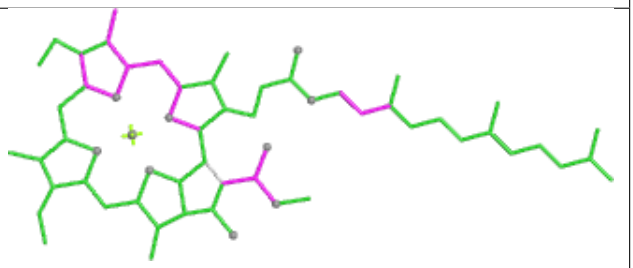


Rings

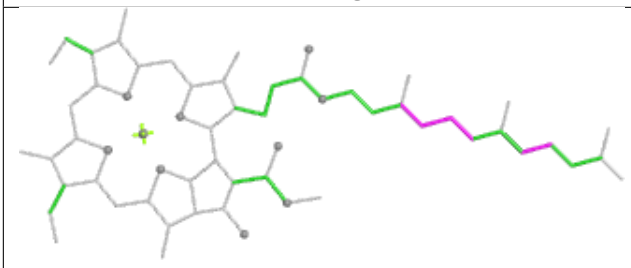
Ligand CLA A 607



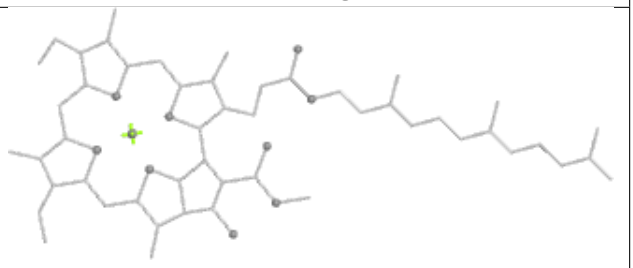
Bond lengths



Bond angles

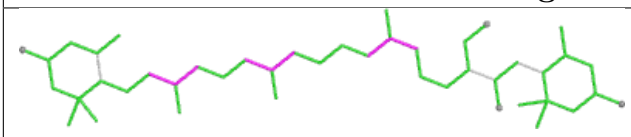


Torsions

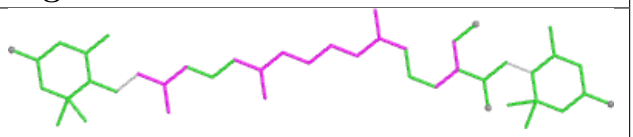


Rings

Ligand 0IE g 303



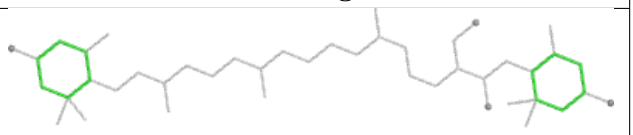
Bond lengths



Bond angles

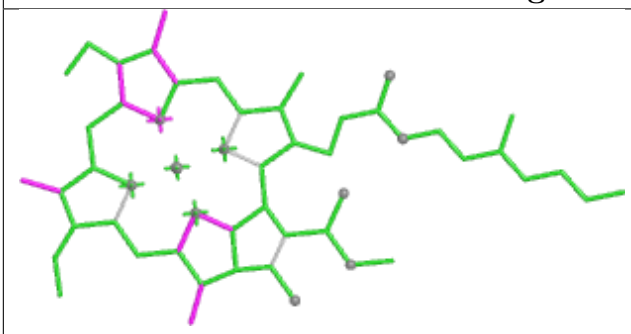


Torsions

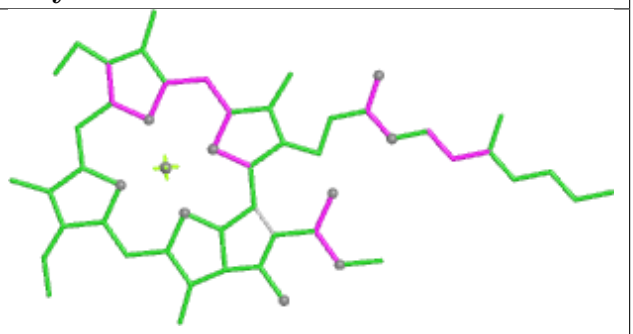


Rings

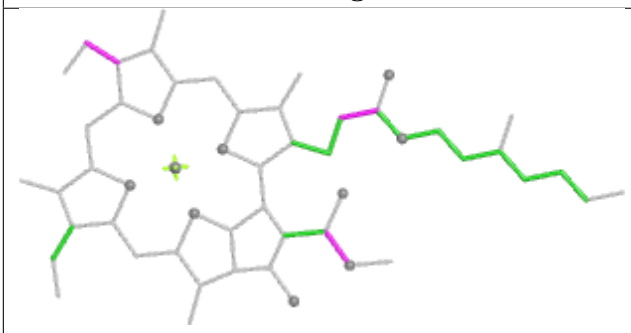
Ligand CLA y 307



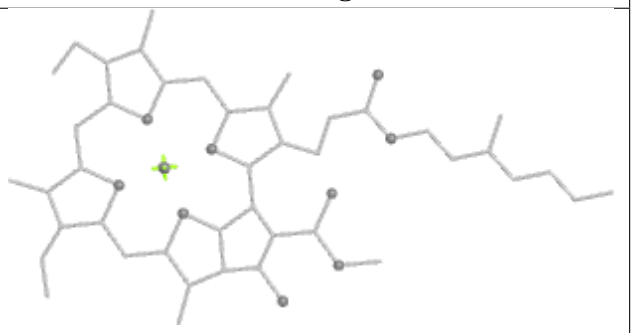
Bond lengths



Bond angles

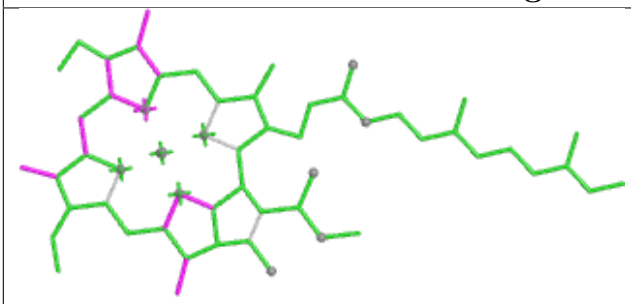


Torsions

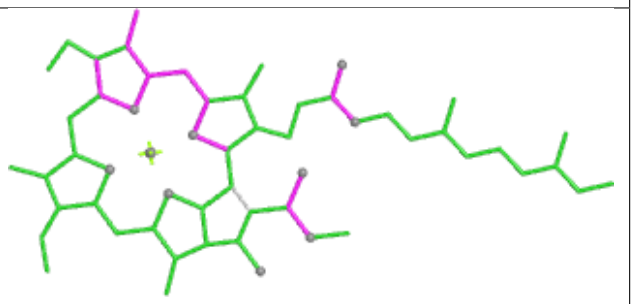


Rings

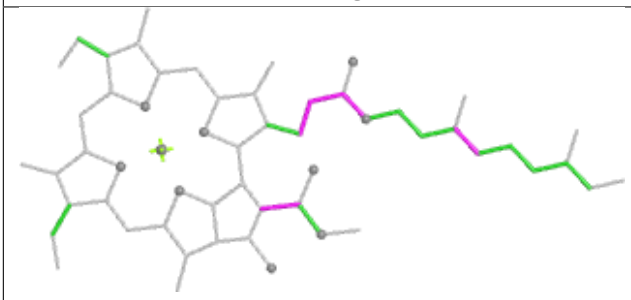
Ligand CLA C 605



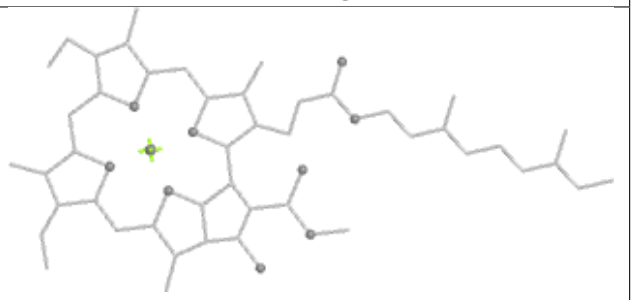
Bond lengths



Bond angles

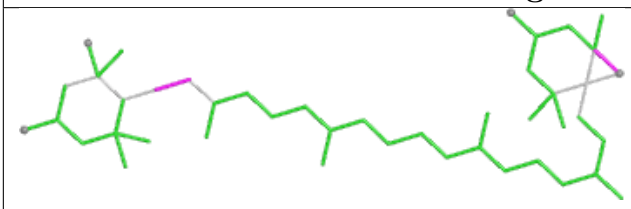


Torsions

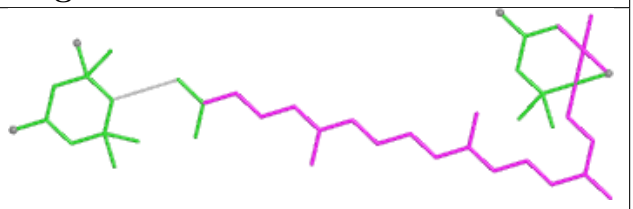


Rings

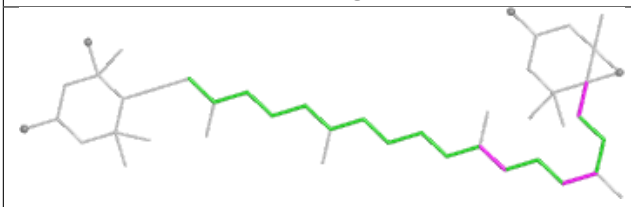
Ligand NEX g 304



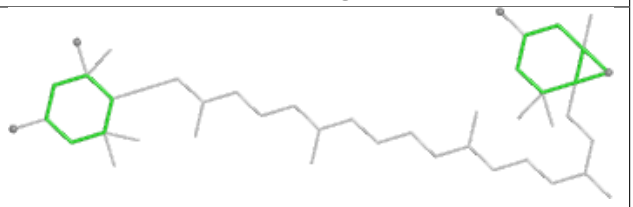
Bond lengths



Bond angles

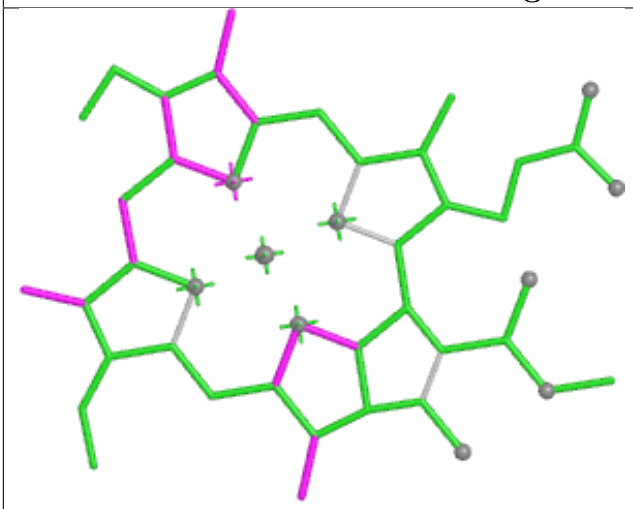


Torsions

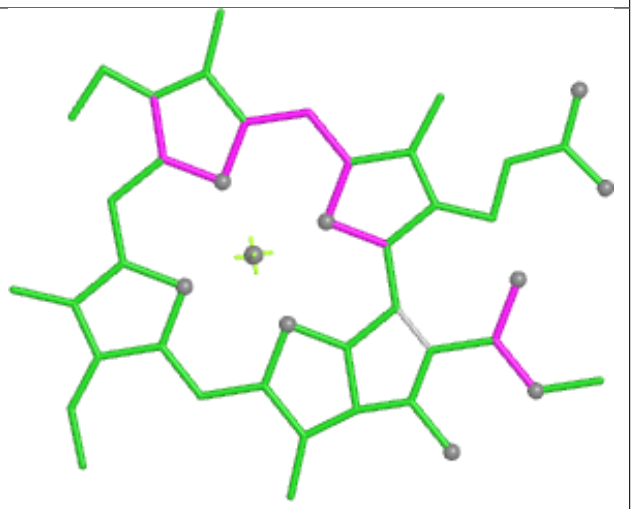


Rings

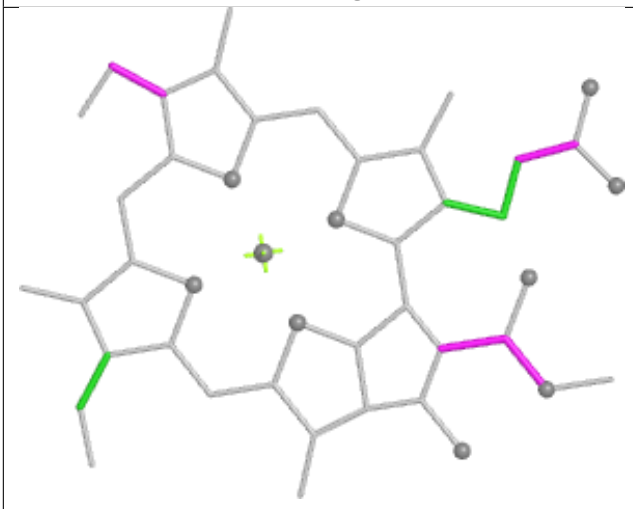
Ligand CLA R 611



Bond lengths



Bond angles

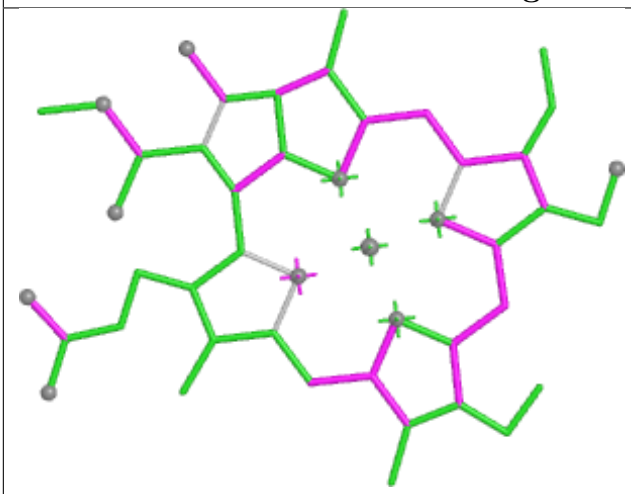


Torsions

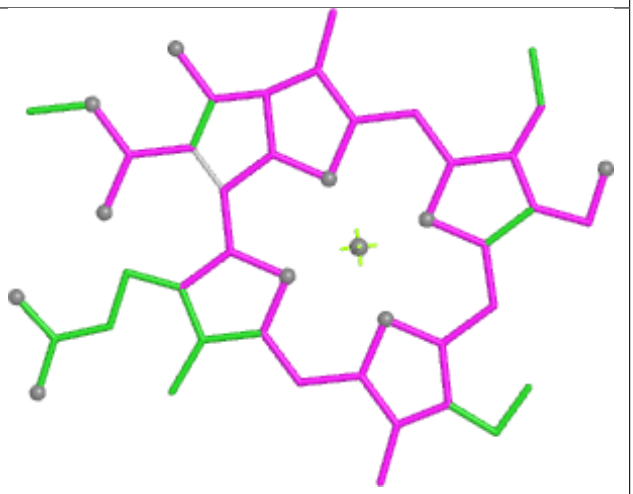


Rings

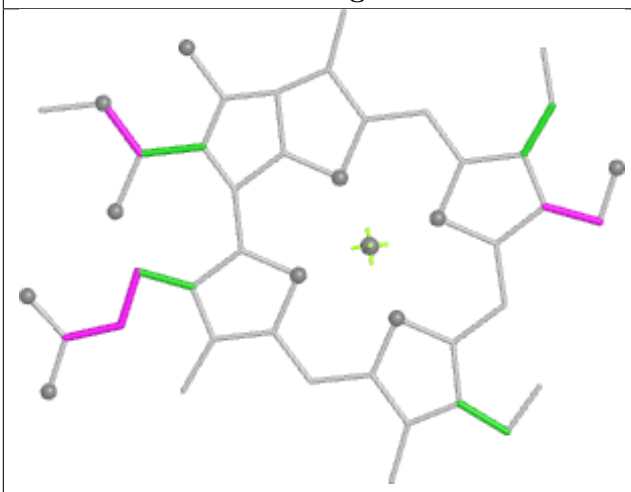
Ligand CHL N 309



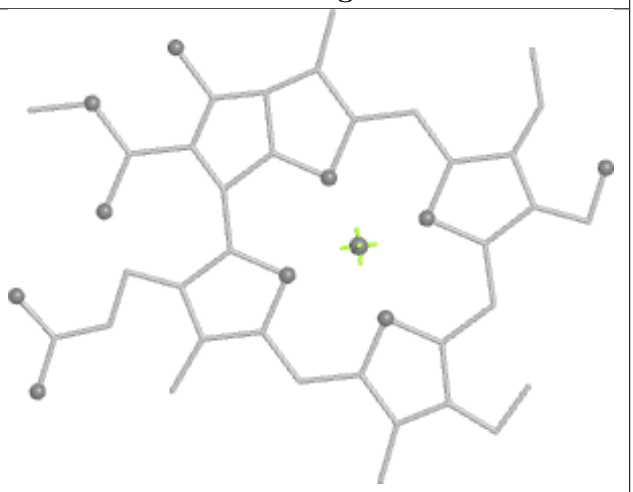
Bond lengths



Bond angles

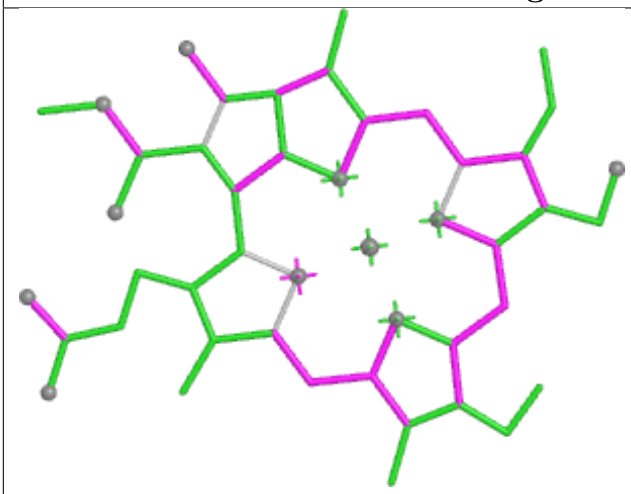


Torsions

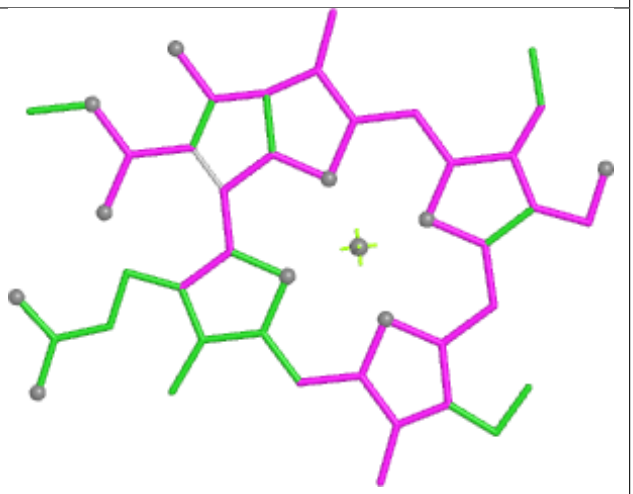


Rings

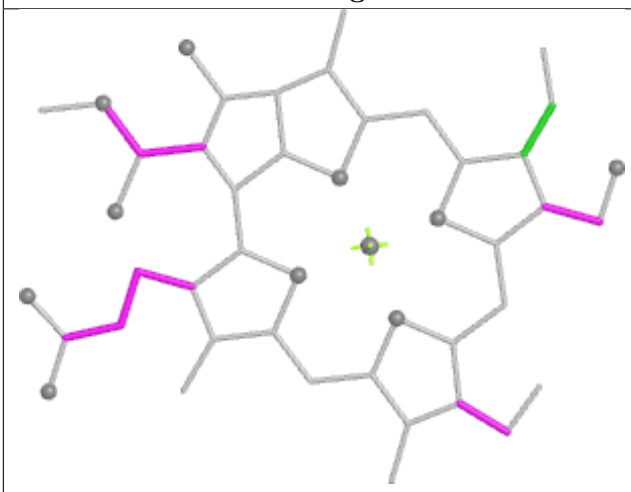
Ligand CHL S 601



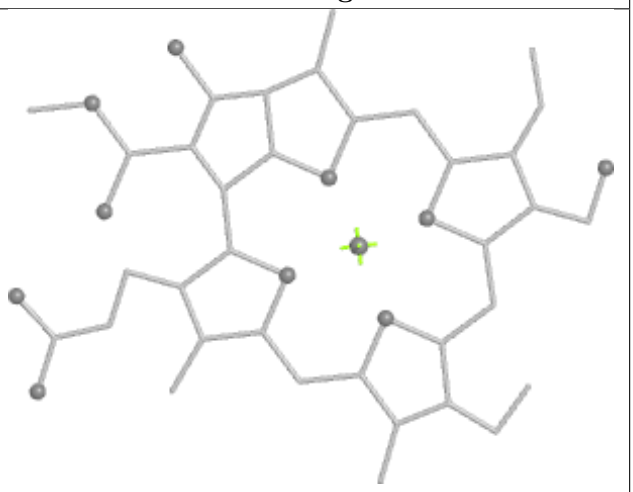
Bond lengths



Bond angles

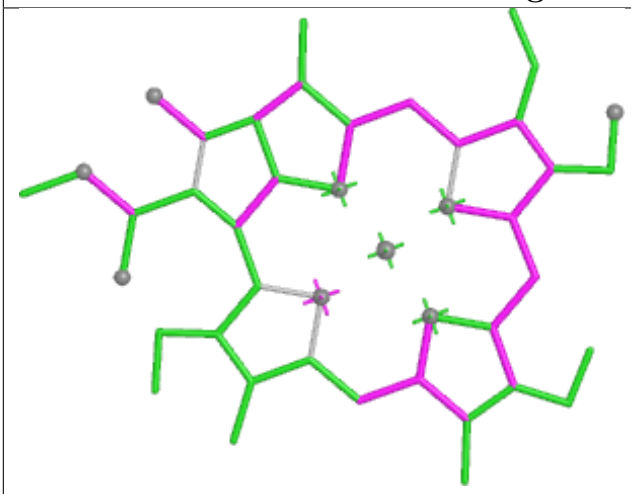


Torsions

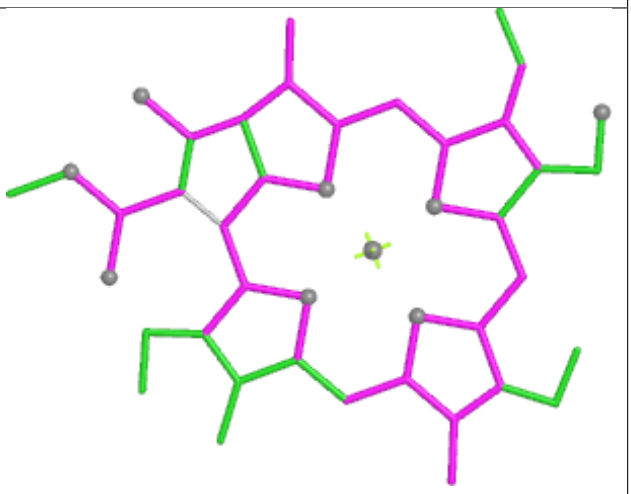


Rings

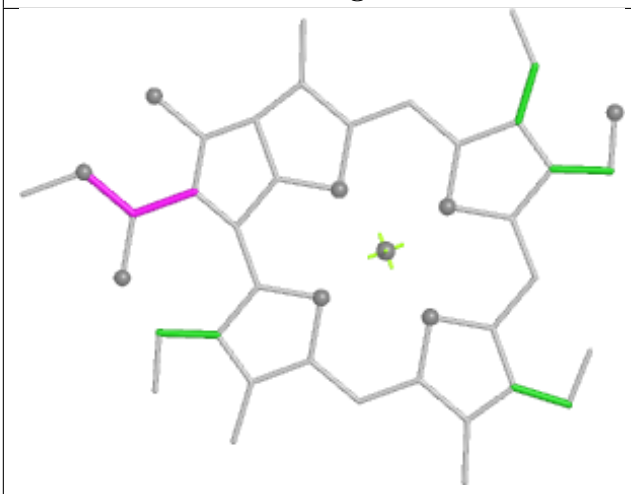
Ligand CHL n 308



Bond lengths



Bond angles

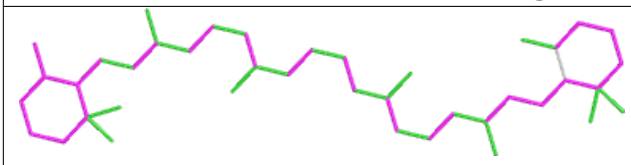


Torsions

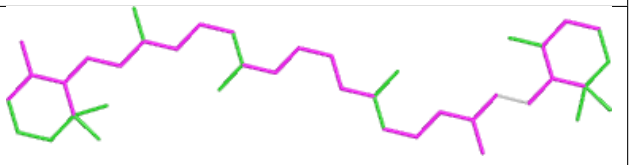


Rings

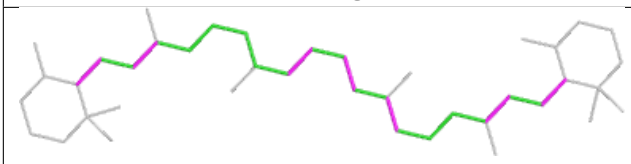
Ligand 8CT v 401



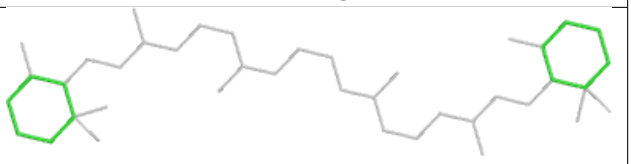
Bond lengths



Bond angles

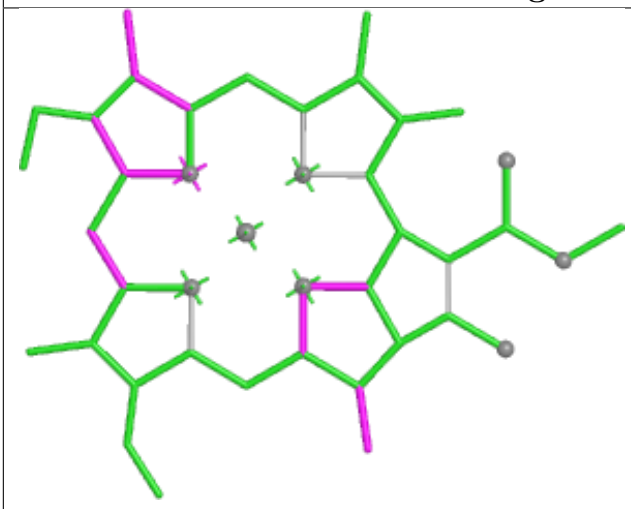


Torsions

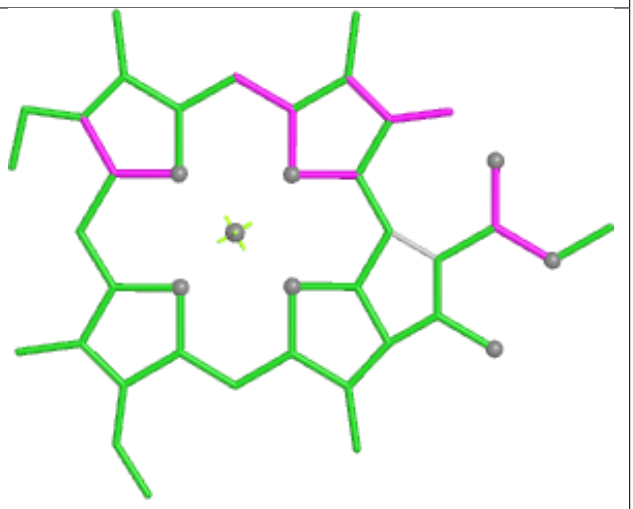


Rings

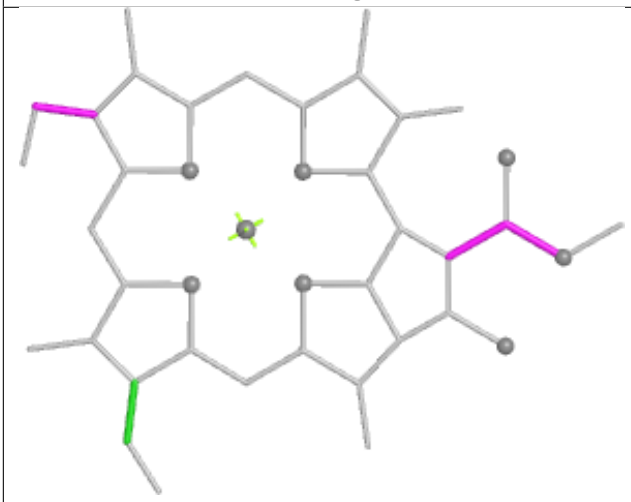
Ligand CLA 3 306



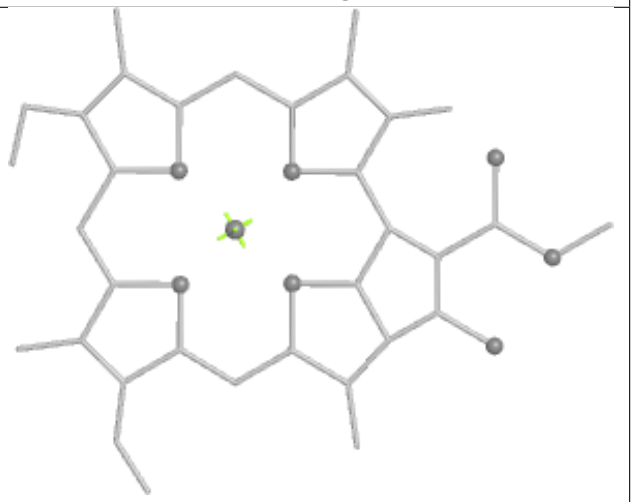
Bond lengths



Bond angles

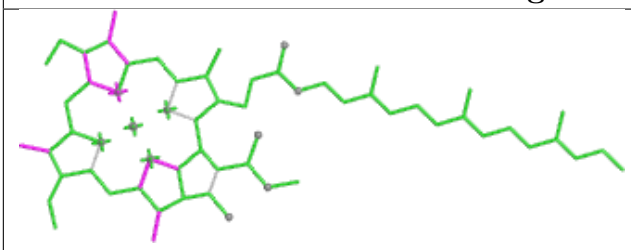


Torsions

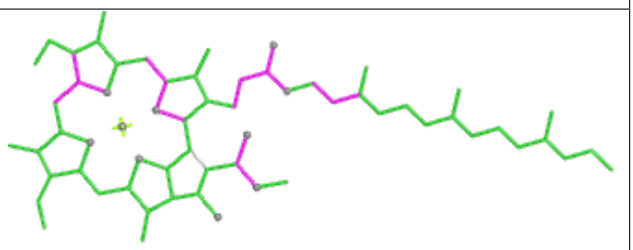


Rings

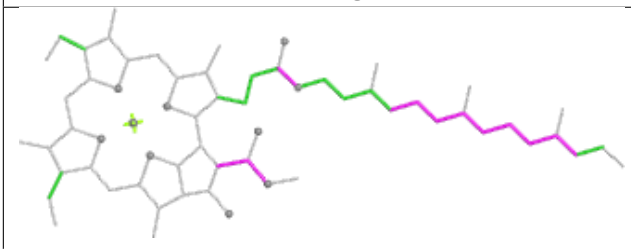
Ligand CLA b 604



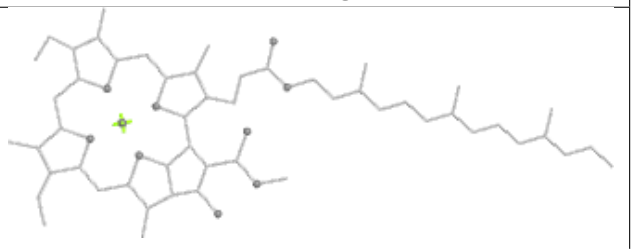
Bond lengths



Bond angles

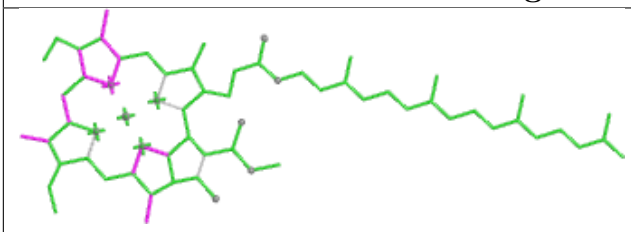


Torsions

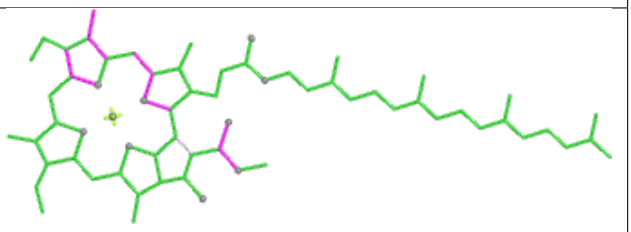


Rings

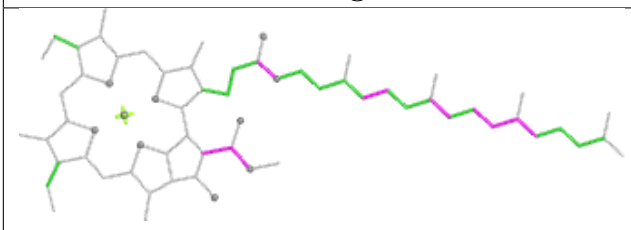
Ligand CLA C 611



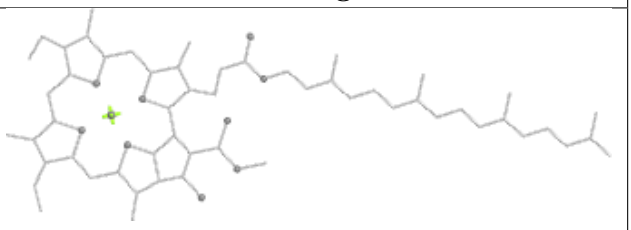
Bond lengths



Bond angles



Torsions

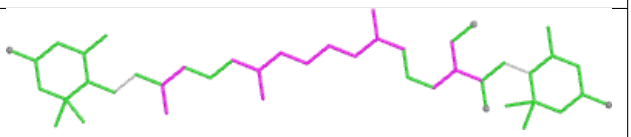


Rings

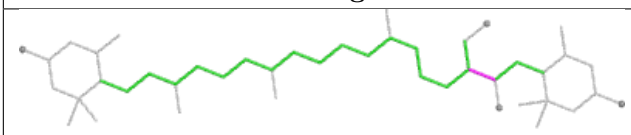
Ligand 0IE 5 302



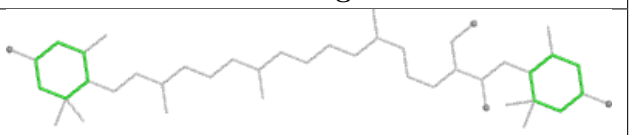
Bond lengths



Bond angles

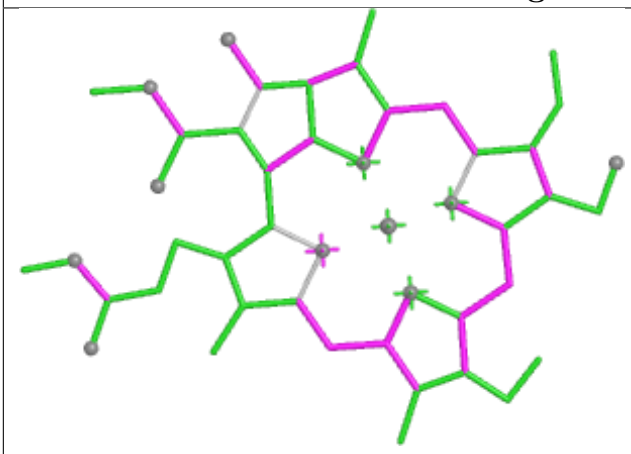


Torsions

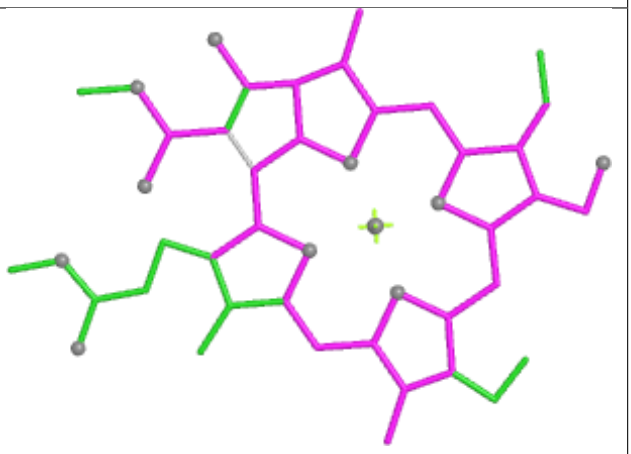


Rings

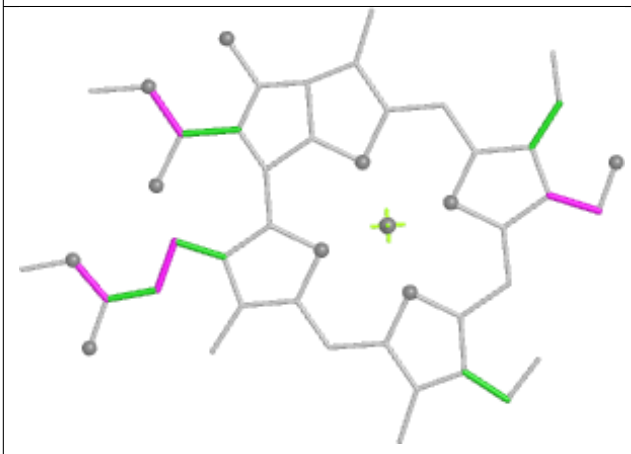
Ligand CHL 7 312



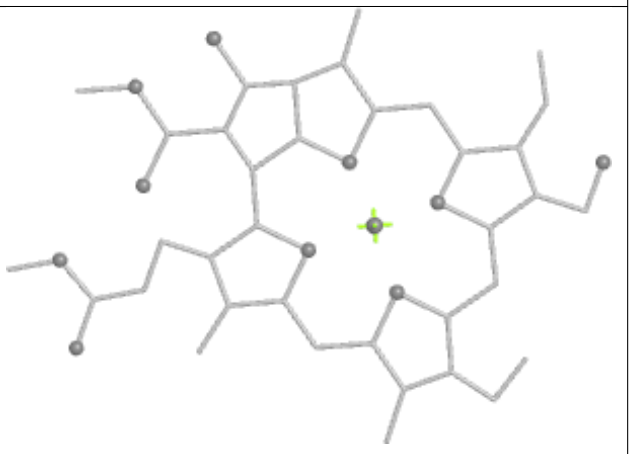
Bond lengths



Bond angles

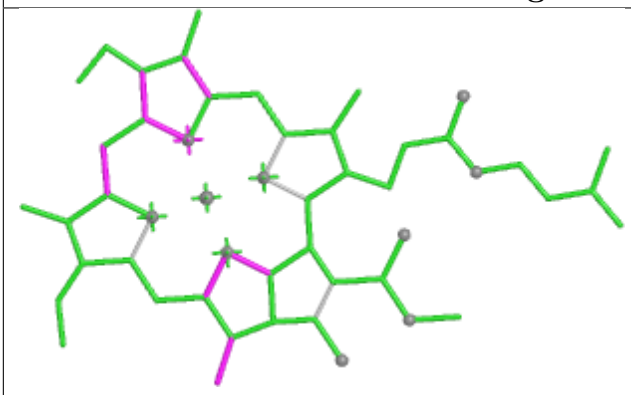


Torsions

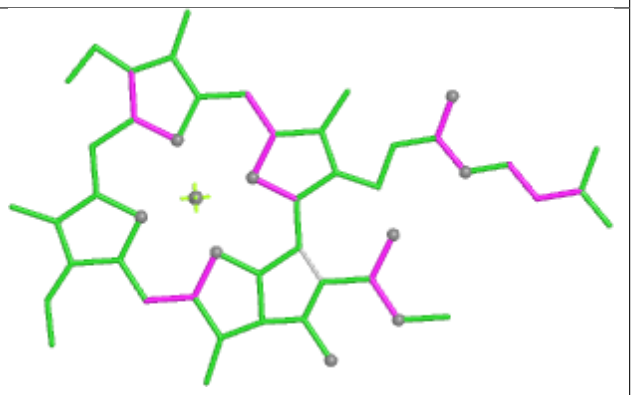


Rings

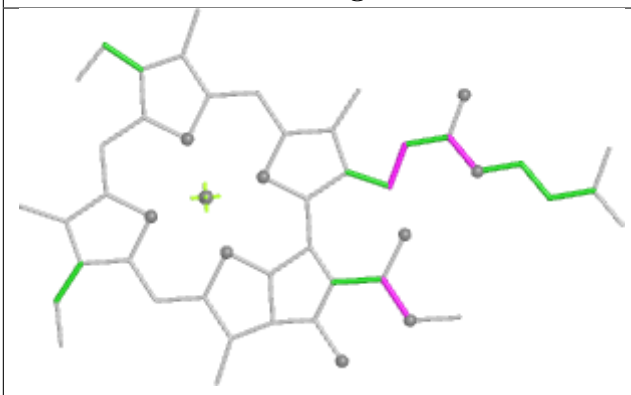
Ligand CLA n 307



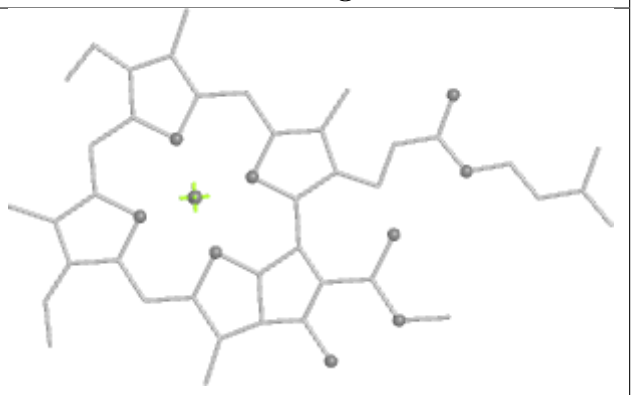
Bond lengths



Bond angles

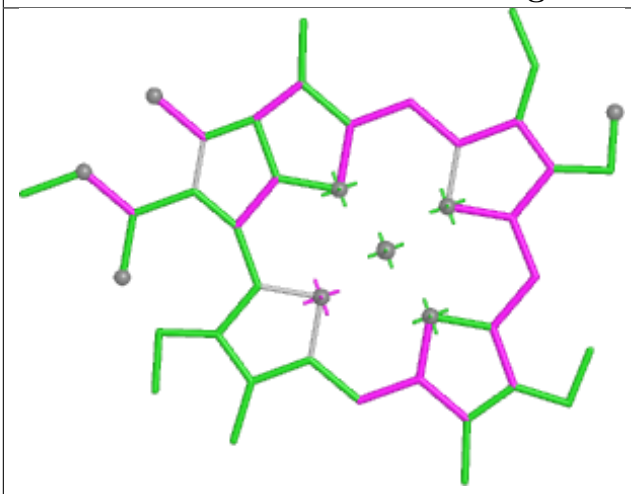


Torsions

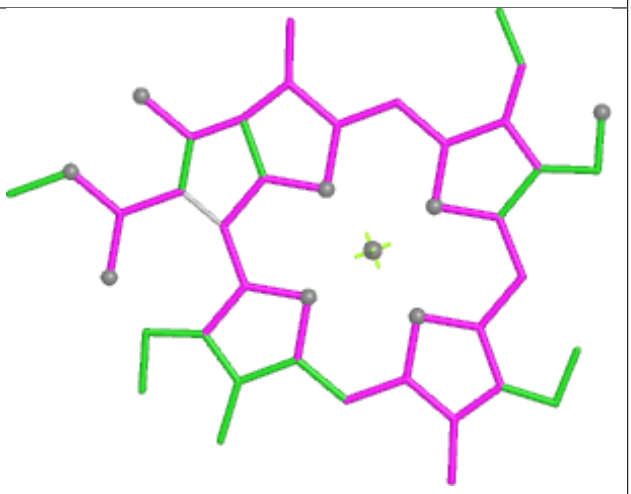


Rings

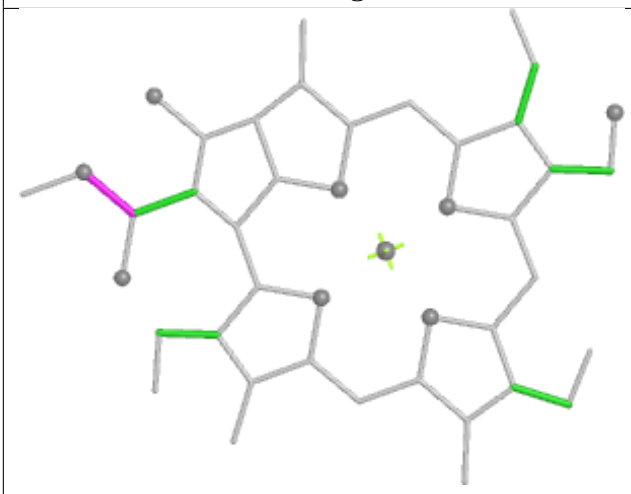
Ligand CHL 4 308



Bond lengths



Bond angles

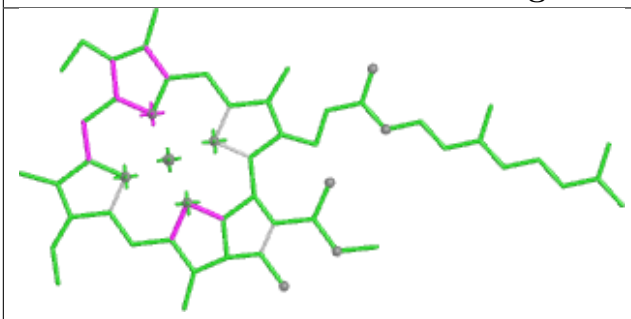


Torsions

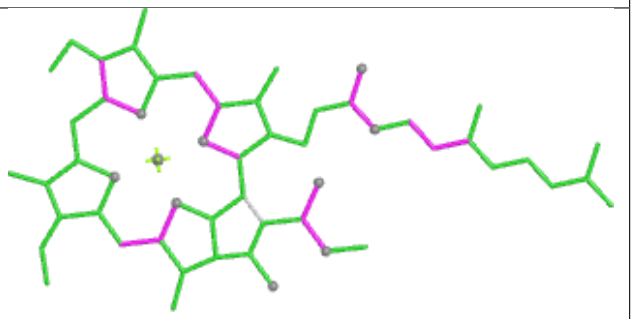


Rings

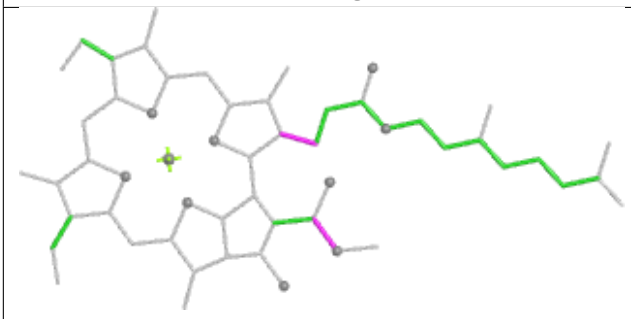
Ligand CLA 9 313



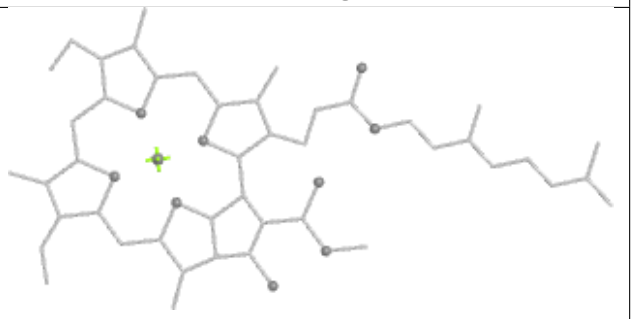
Bond lengths



Bond angles

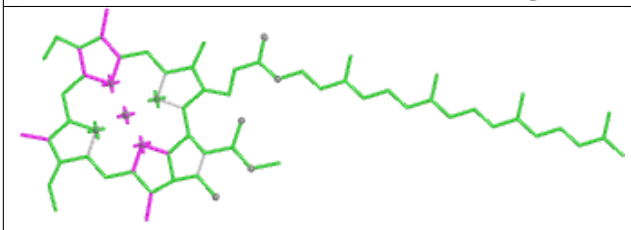


Torsions

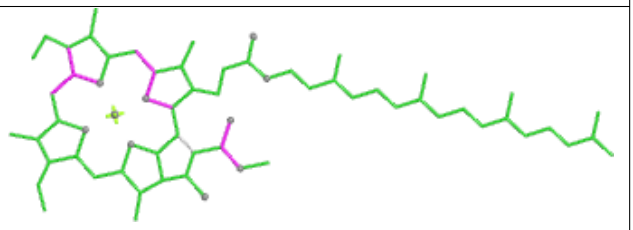


Rings

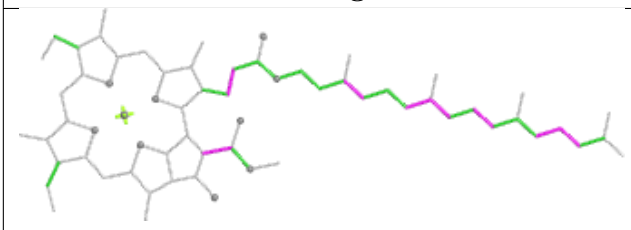
Ligand CLA C 607



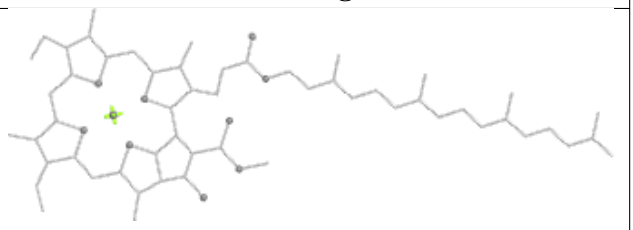
Bond lengths



Bond angles

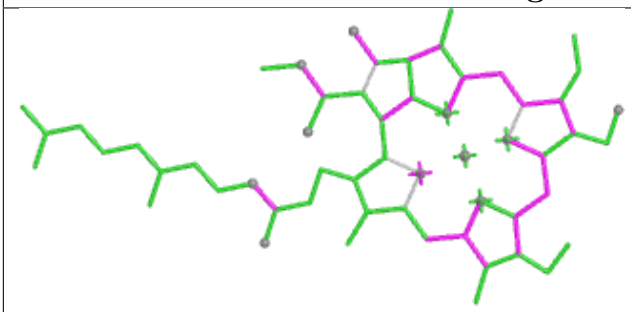


Torsions

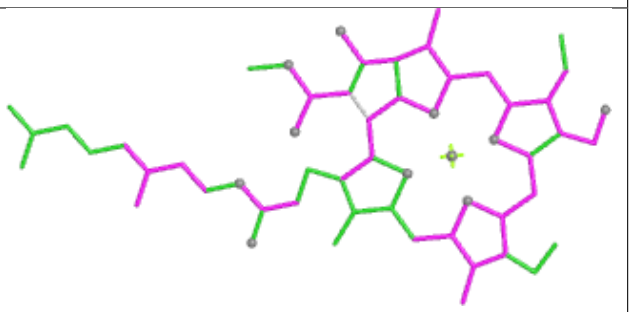


Rings

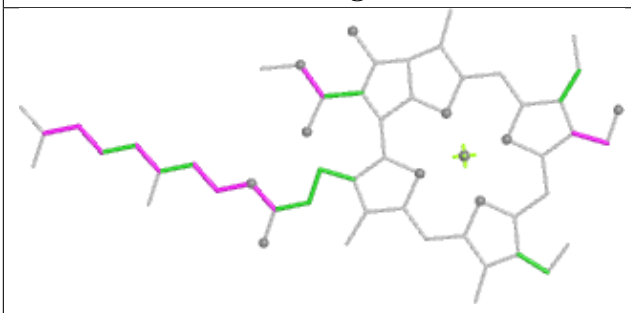
Ligand CHL n 312



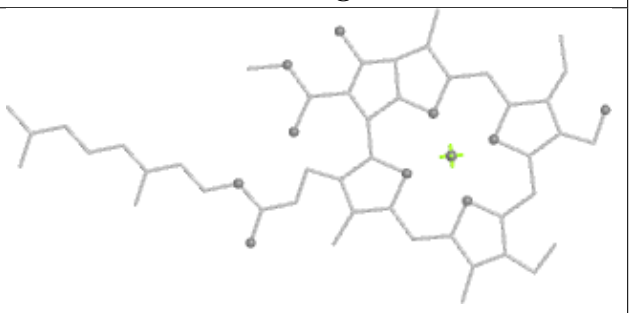
Bond lengths



Bond angles

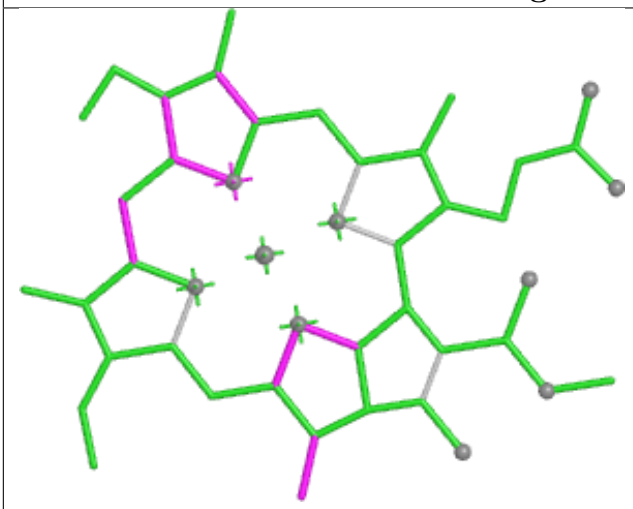


Torsions

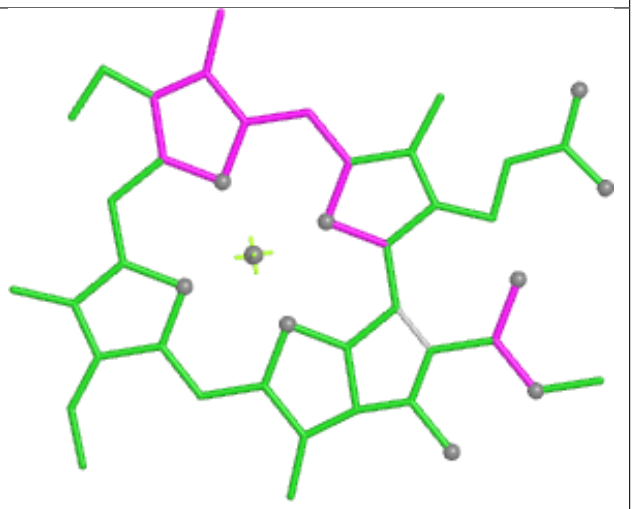


Rings

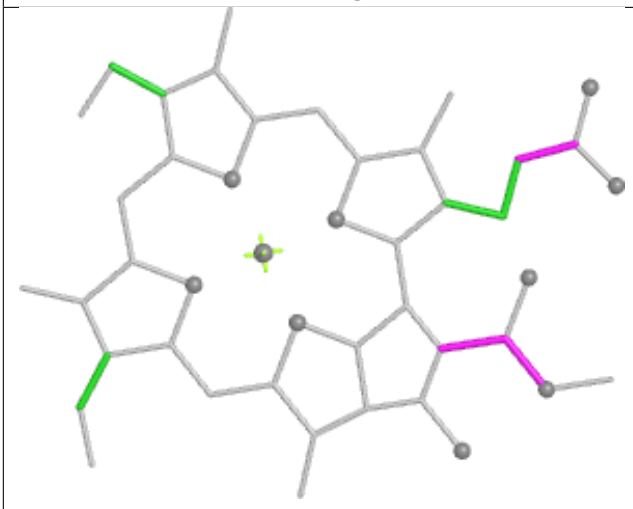
Ligand CLA r 311



Bond lengths



Bond angles

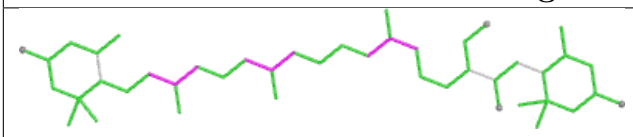


Torsions

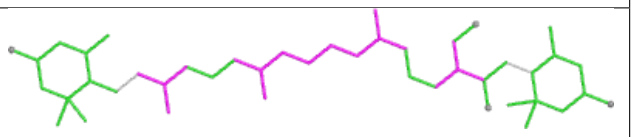


Rings

Ligand 0IE 1 302



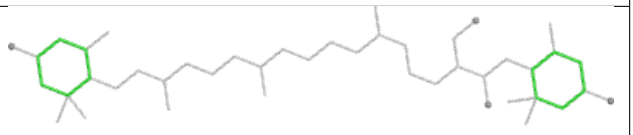
Bond lengths



Bond angles

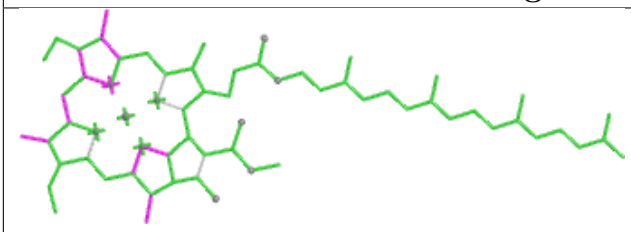


Torsions

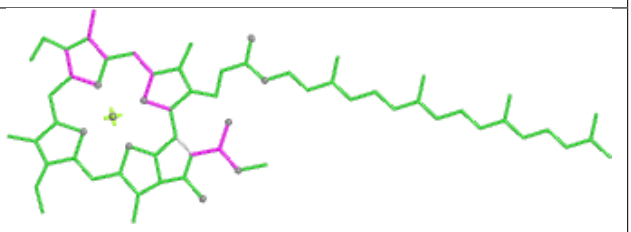


Rings

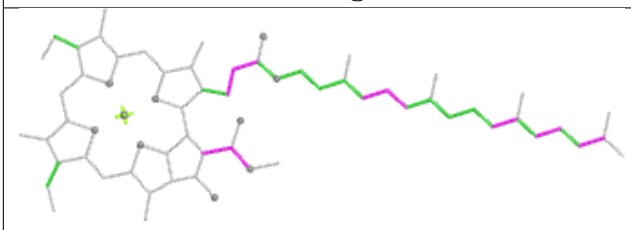
Ligand CLA B 602



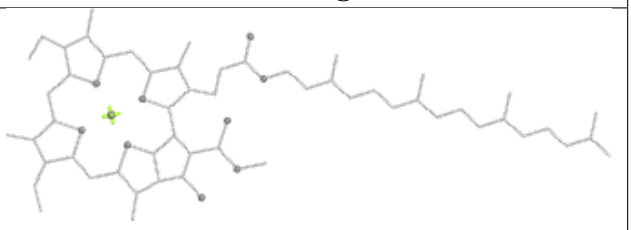
Bond lengths



Bond angles

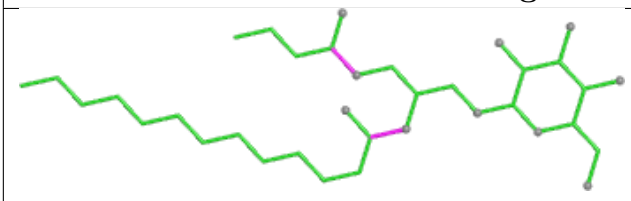


Torsions



Rings

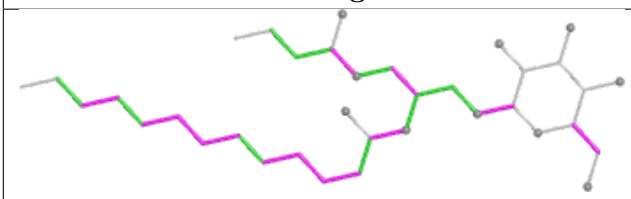
Ligand LMG w 201



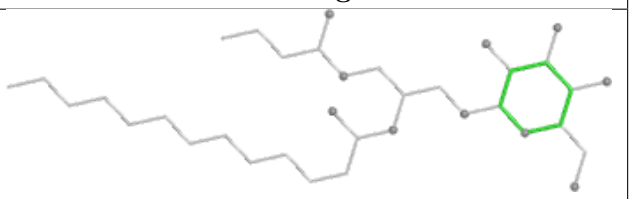
Bond lengths



Bond angles

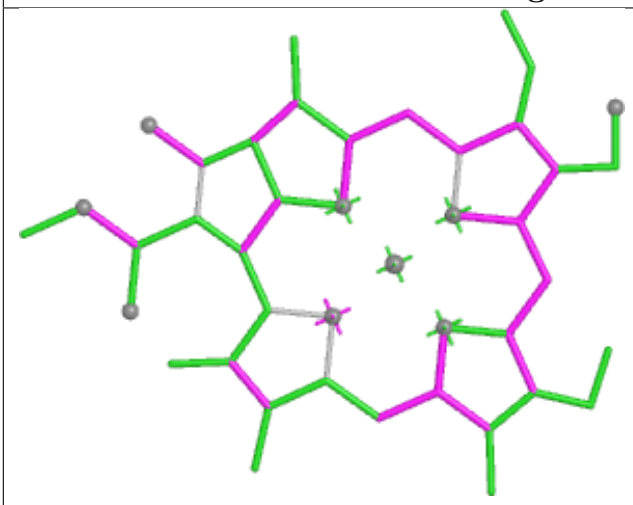


Torsions

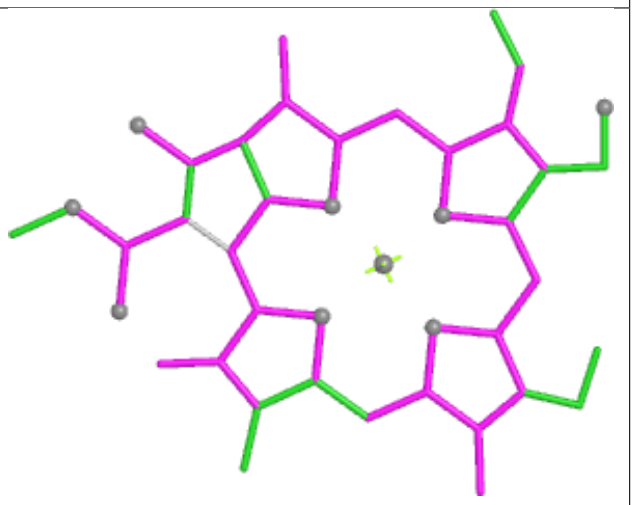


Rings

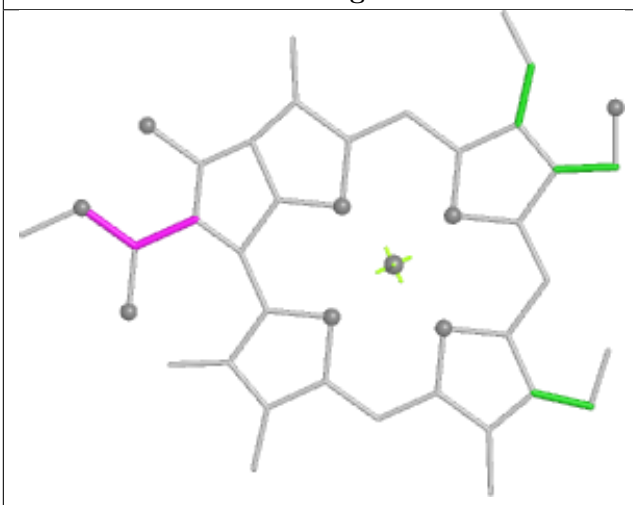
Ligand CHL 9 317



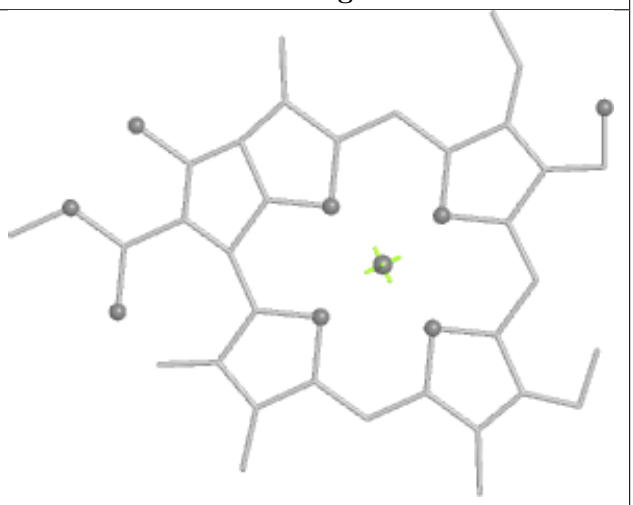
Bond lengths



Bond angles

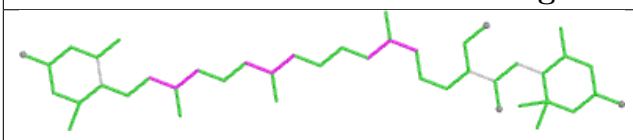


Torsions

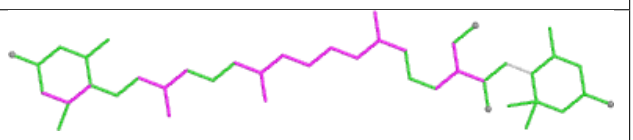


Rings

Ligand 0IE 6 302



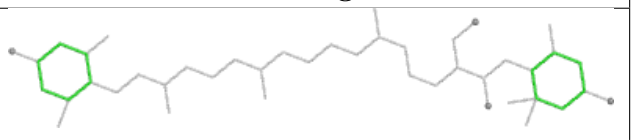
Bond lengths



Bond angles

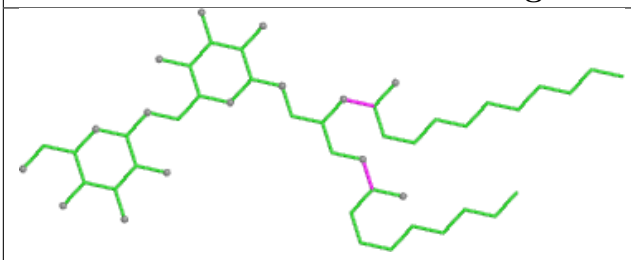


Torsions

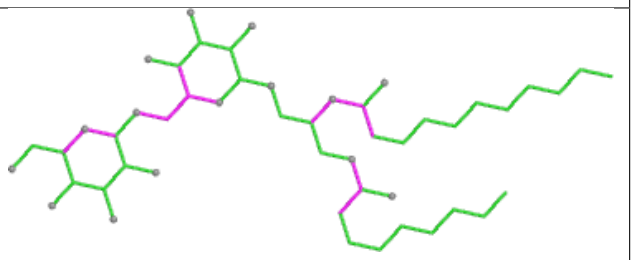


Rings

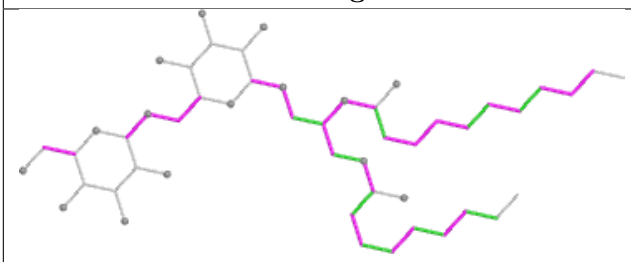
Ligand DGD c 618



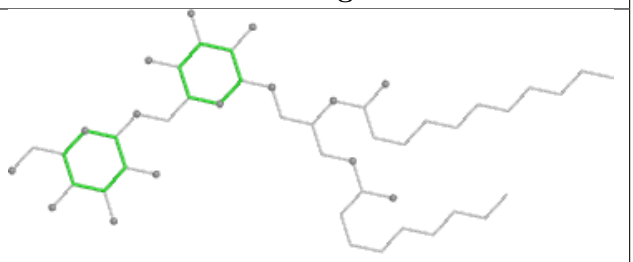
Bond lengths



Bond angles

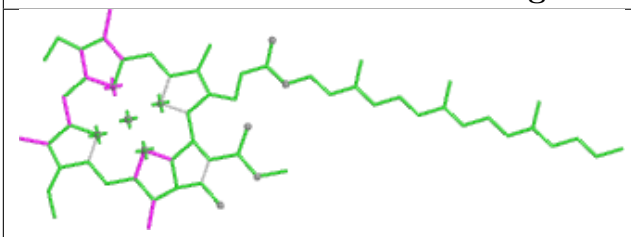


Torsions

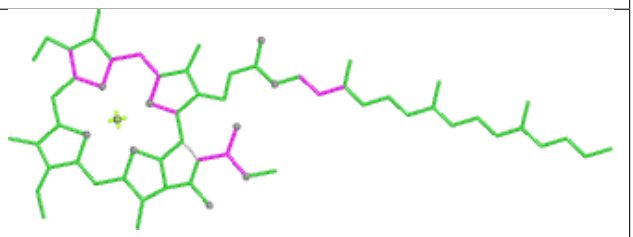


Rings

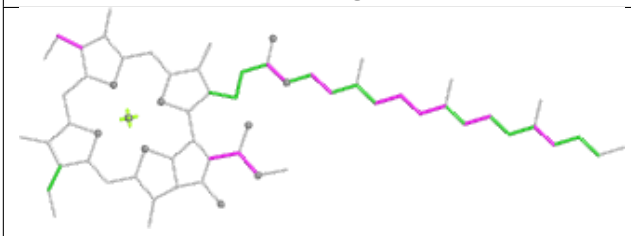
Ligand CLA 7 315



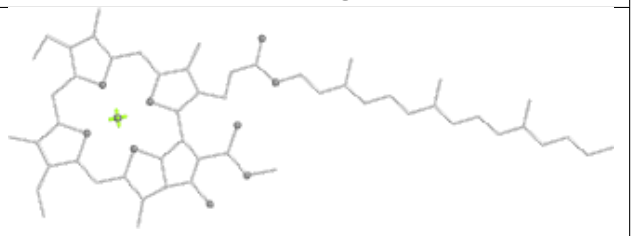
Bond lengths



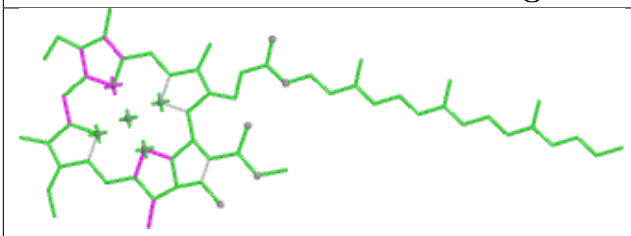
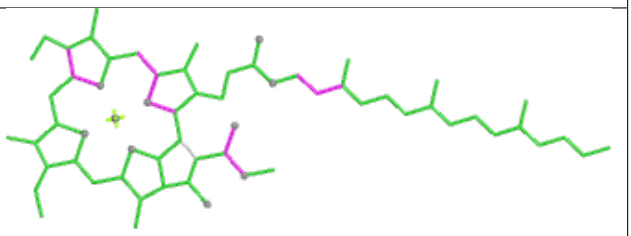
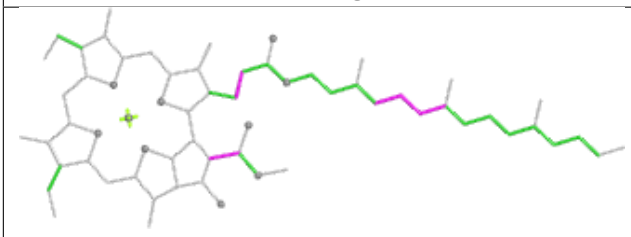
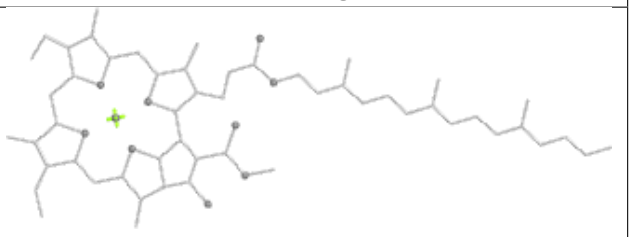
Bond angles

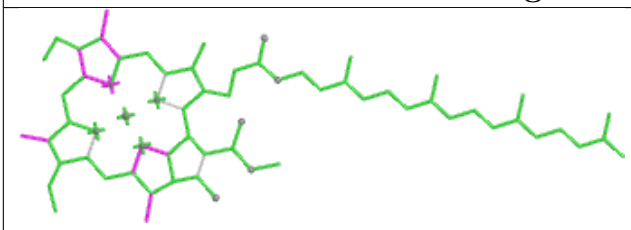
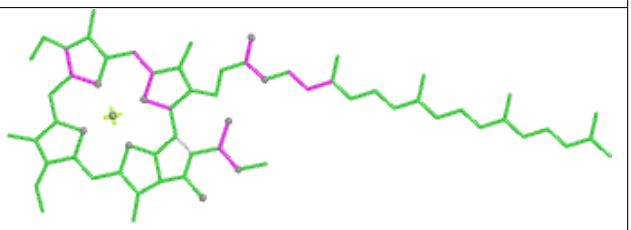
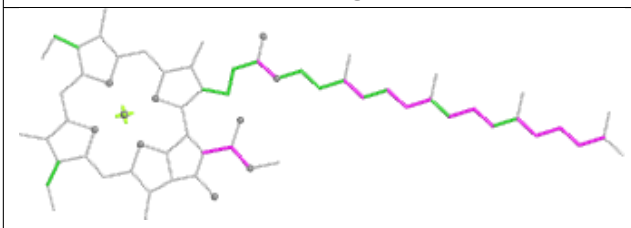
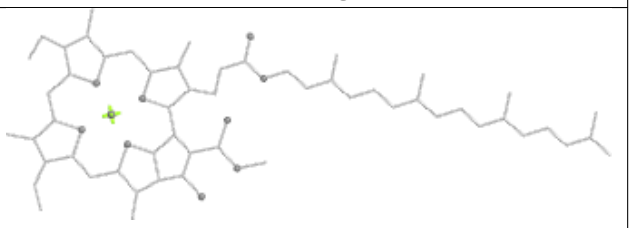


Torsions

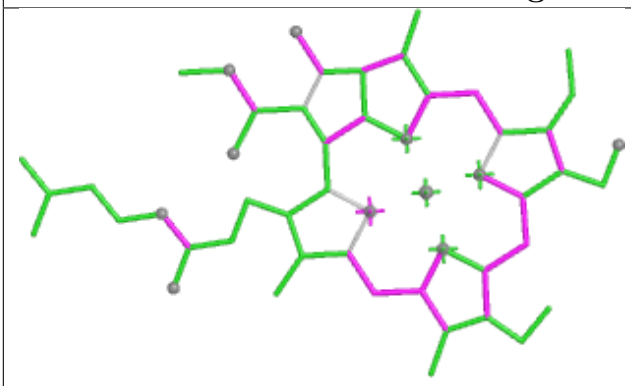


Rings

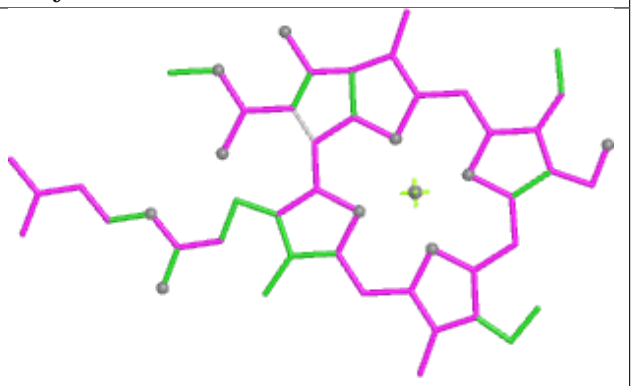
Ligand CLA N 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

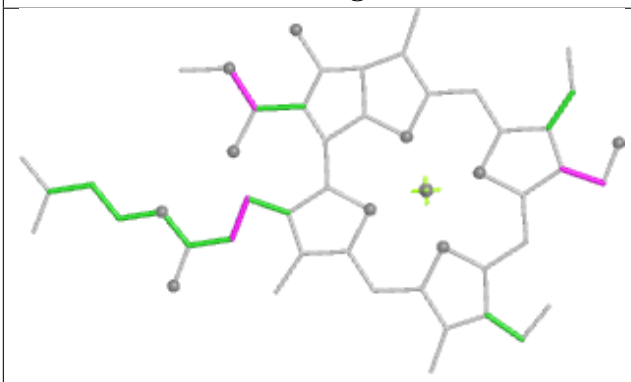
Ligand CHL y 312



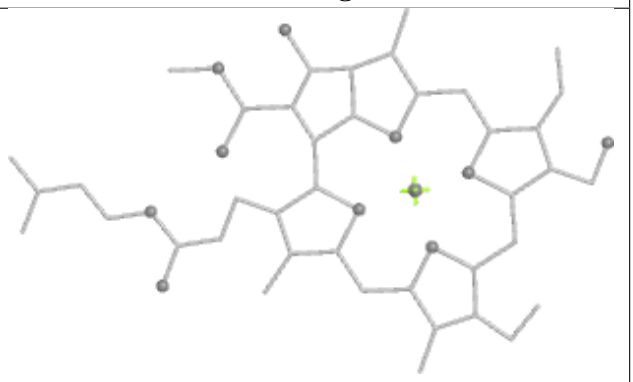
Bond lengths



Bond angles

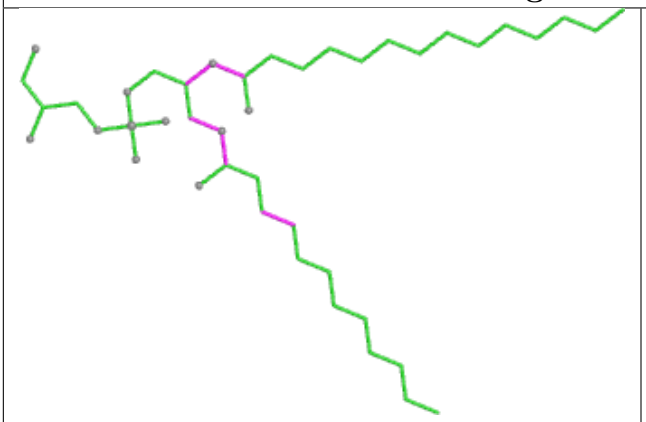


Torsions

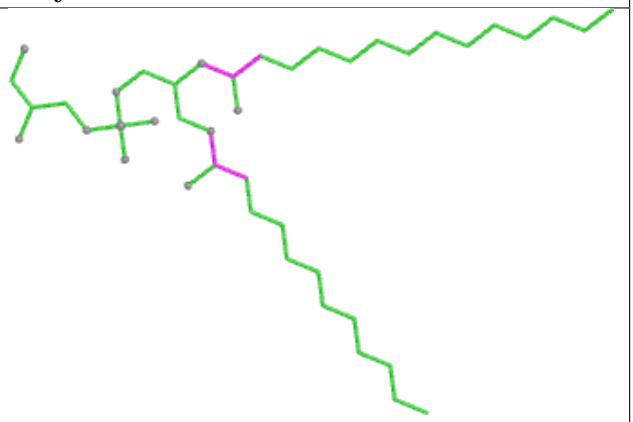


Rings

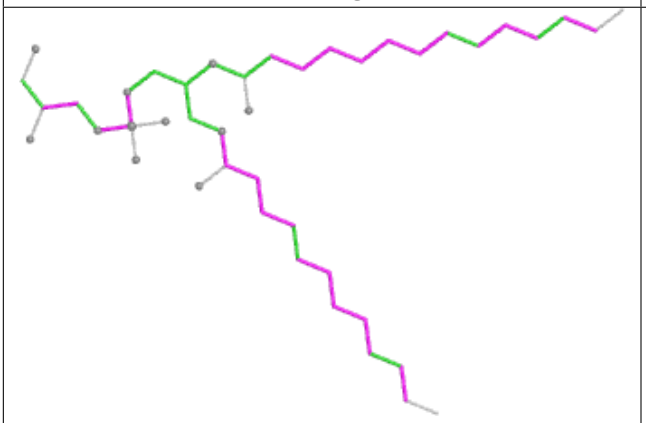
Ligand LHG y 319



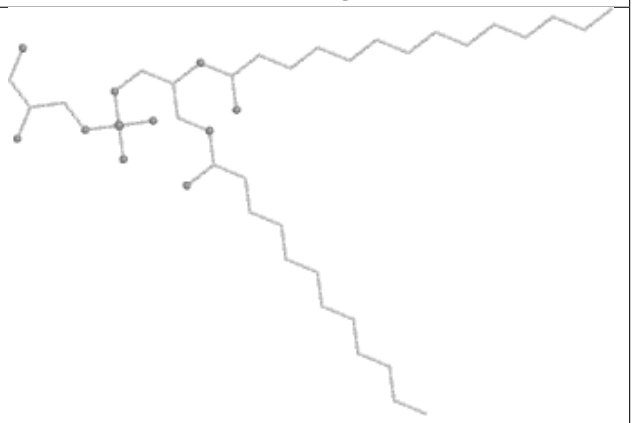
Bond lengths



Bond angles

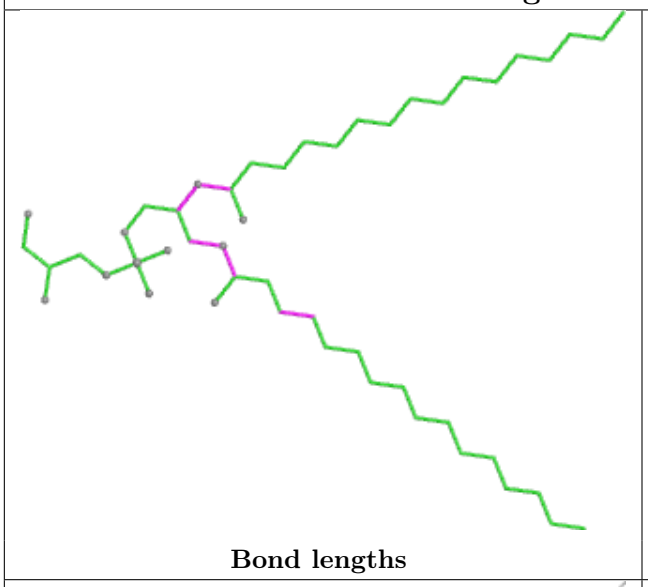


Torsions

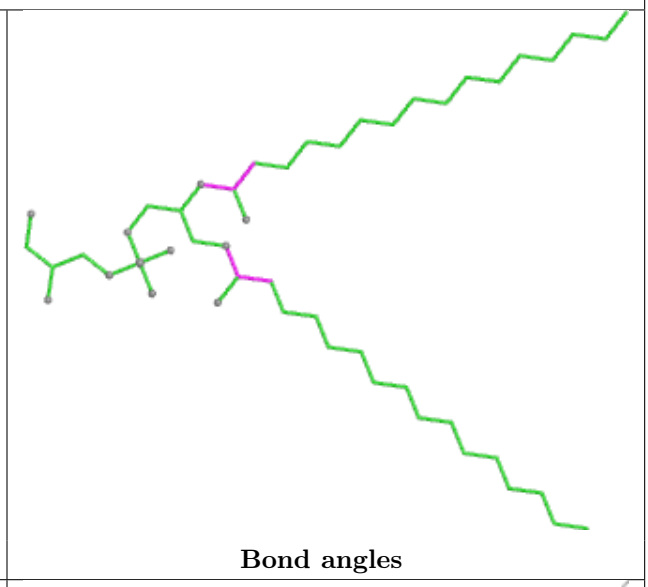


Rings

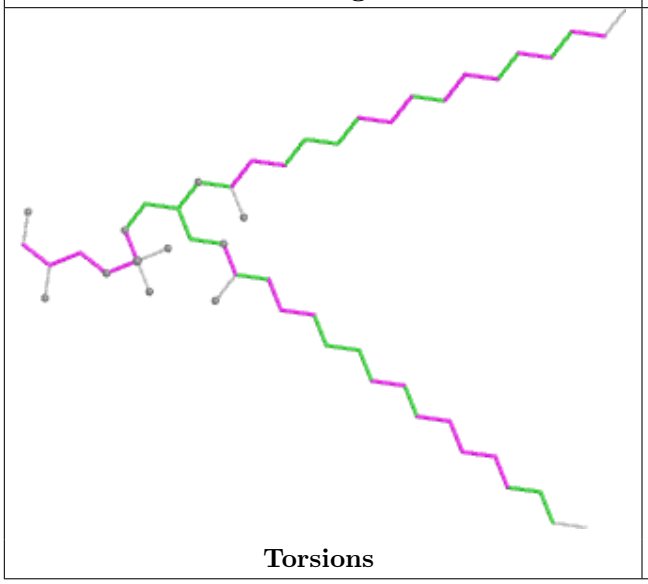
Ligand LHG D 407



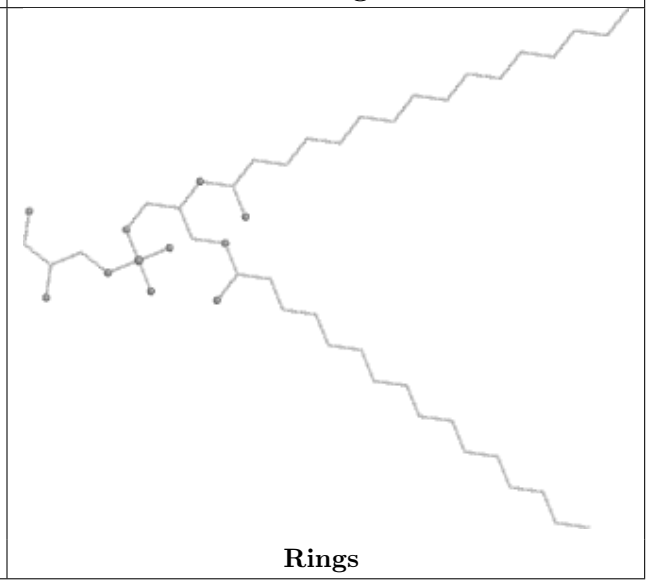
Bond lengths



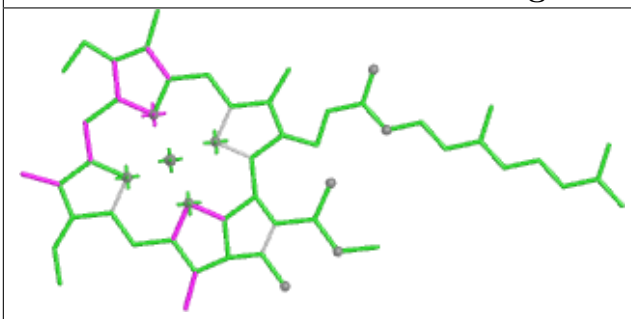
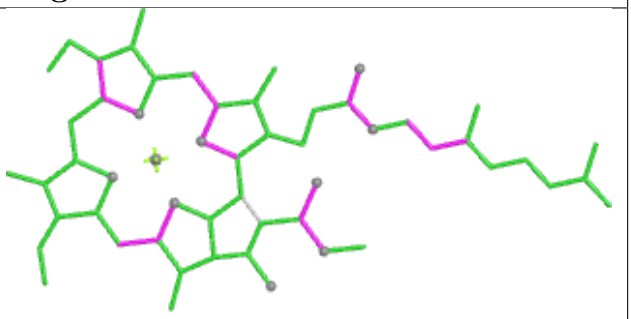
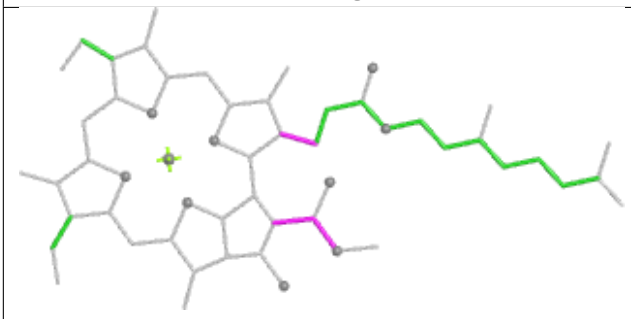
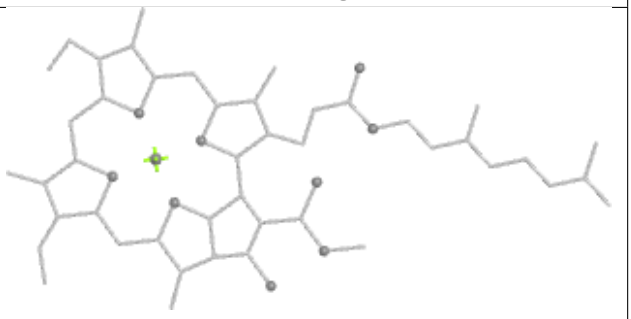
Bond angles

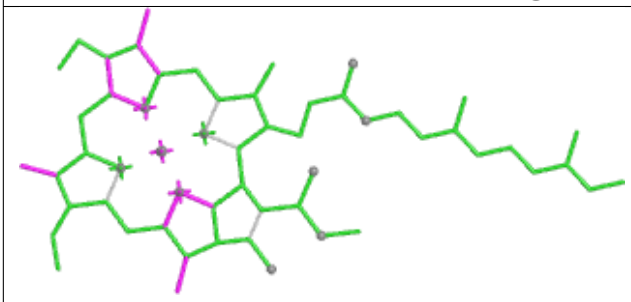
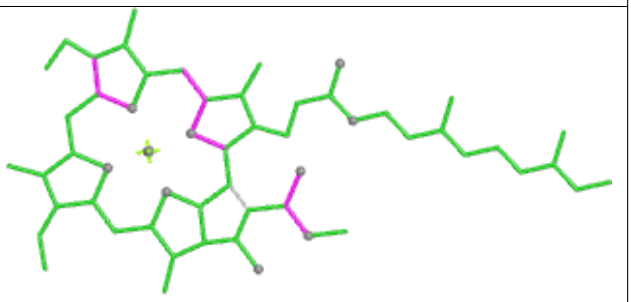
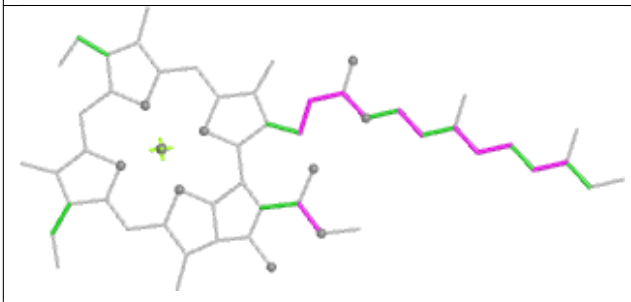
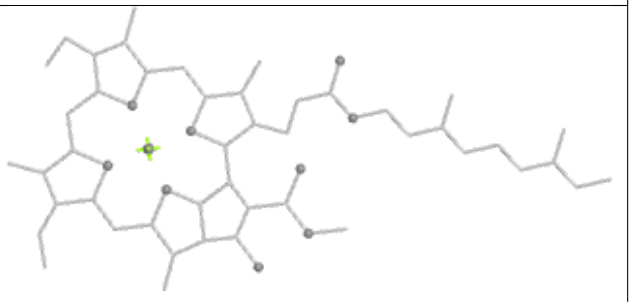


Torsions

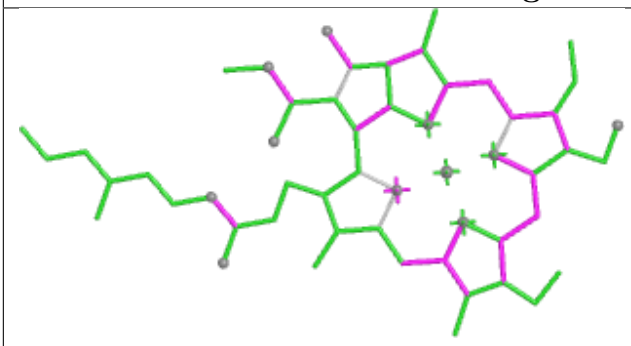


Rings

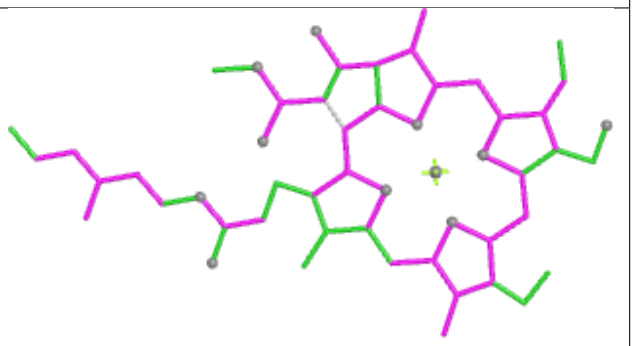
Ligand CLA g 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

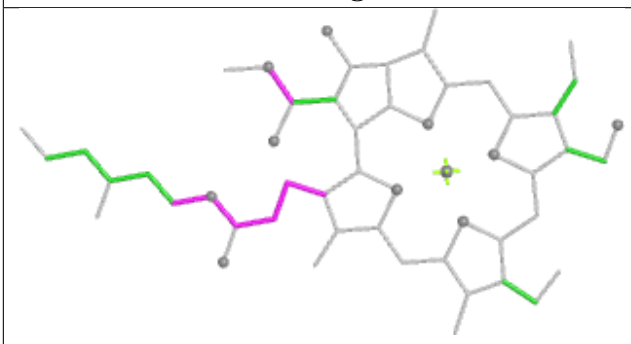
Ligand CHL N 310



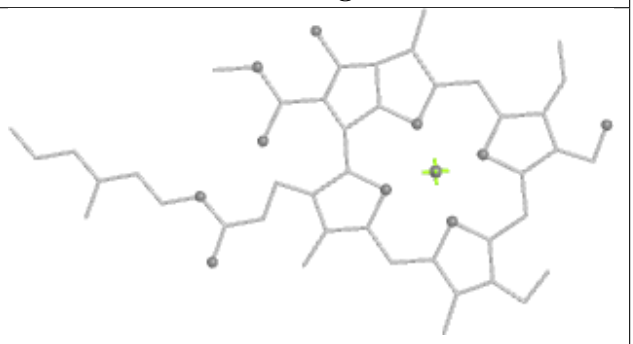
Bond lengths



Bond angles

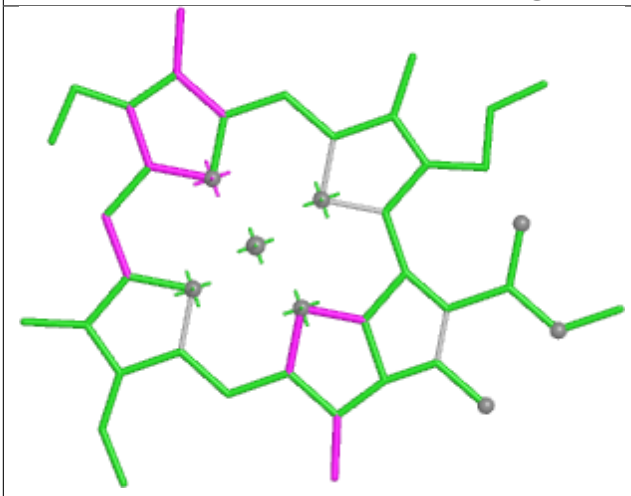


Torsions

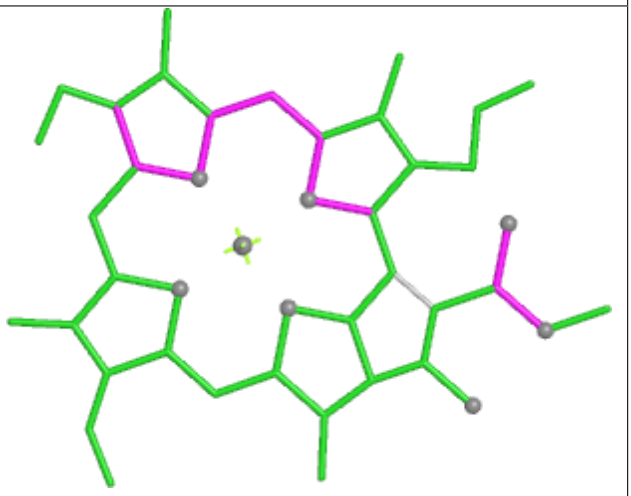


Rings

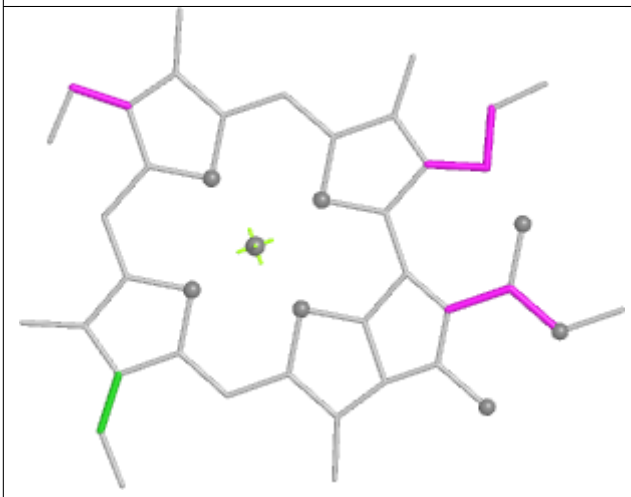
Ligand CLA 5 307



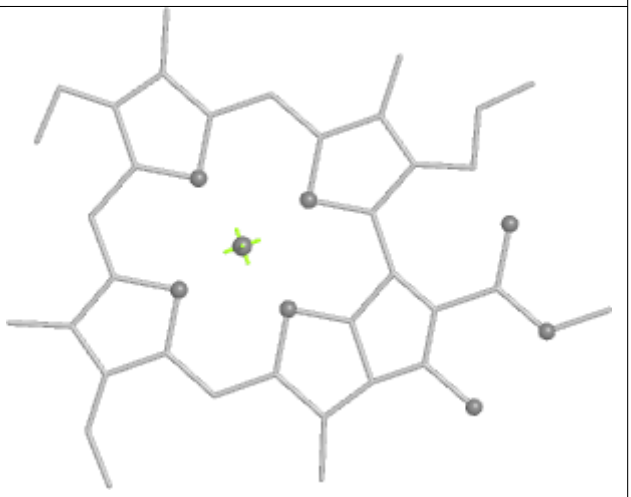
Bond lengths



Bond angles

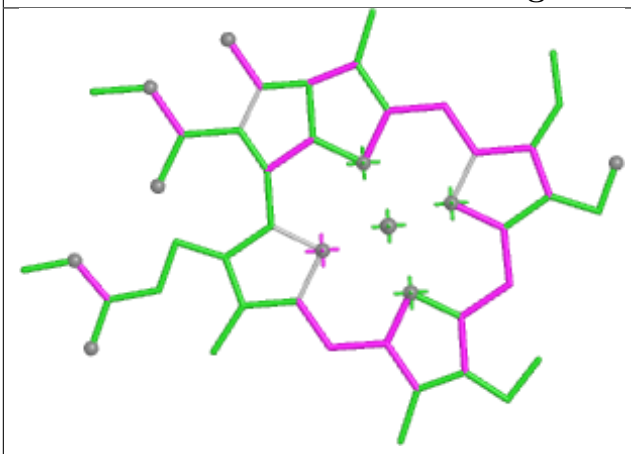


Torsions

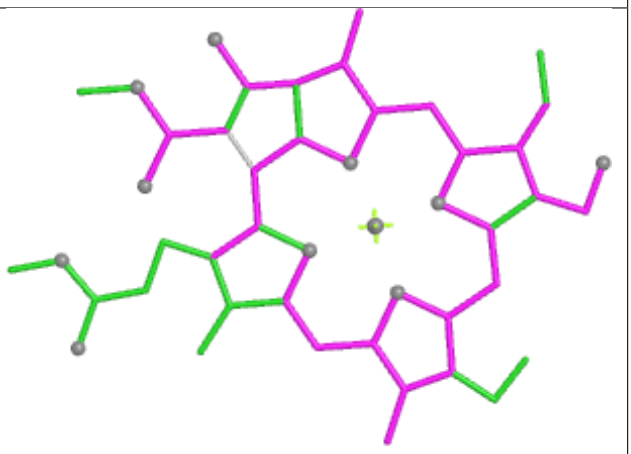


Rings

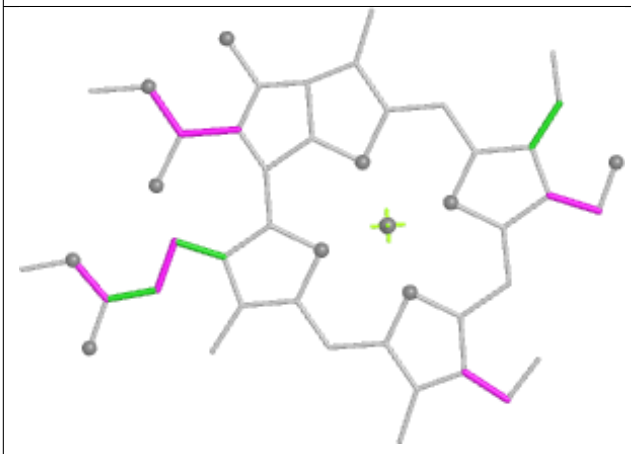
Ligand CHL 2 306



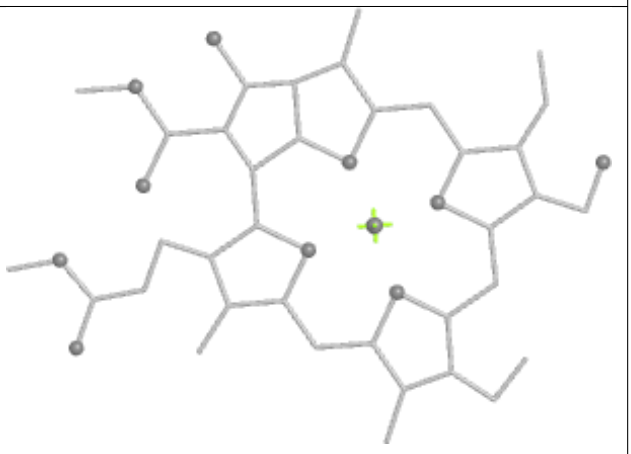
Bond lengths



Bond angles

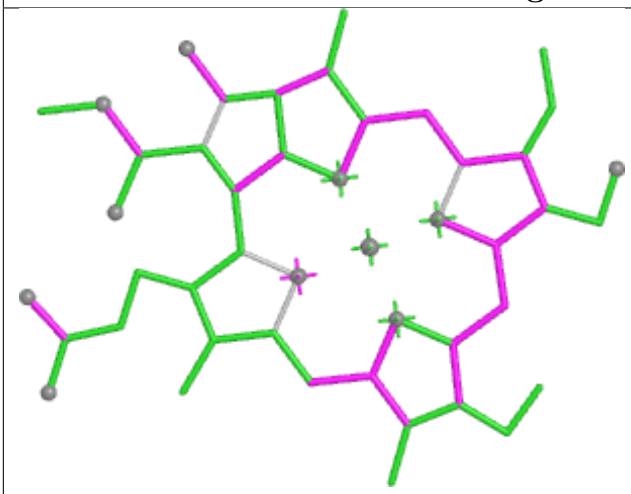


Torsions

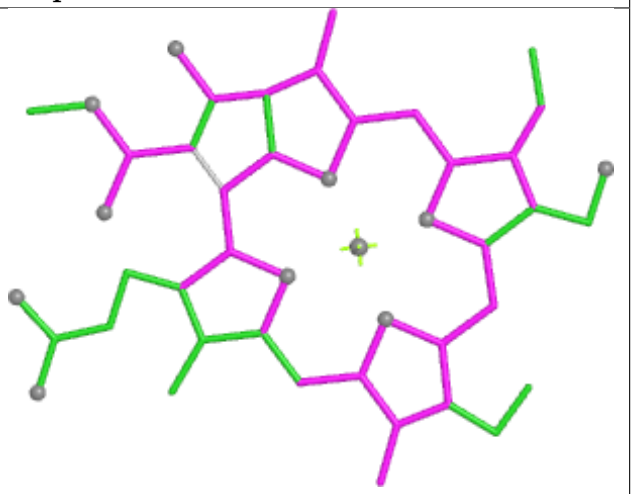


Rings

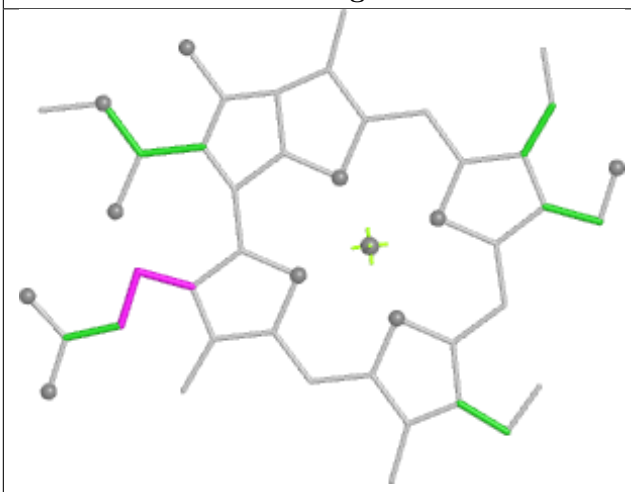
Ligand CHL p 311



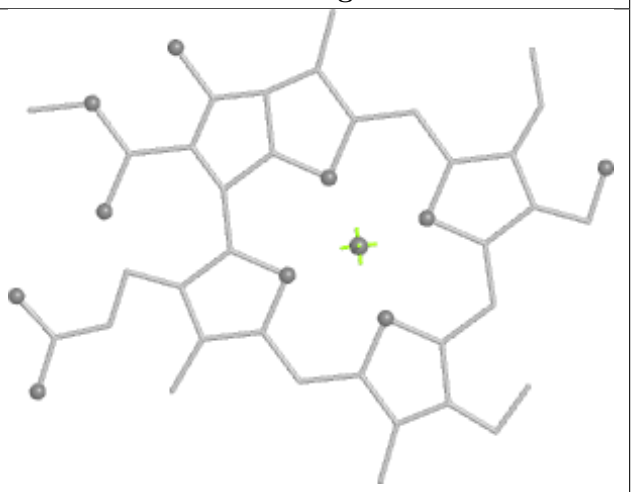
Bond lengths



Bond angles

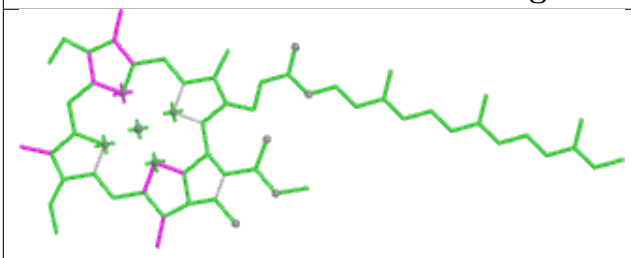


Torsions

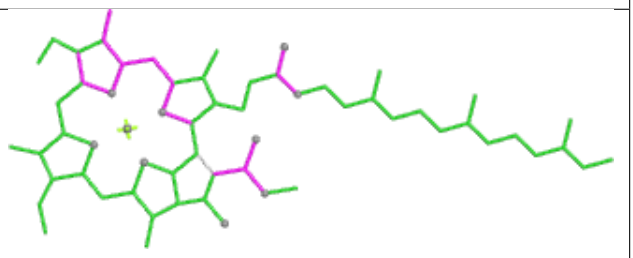


Rings

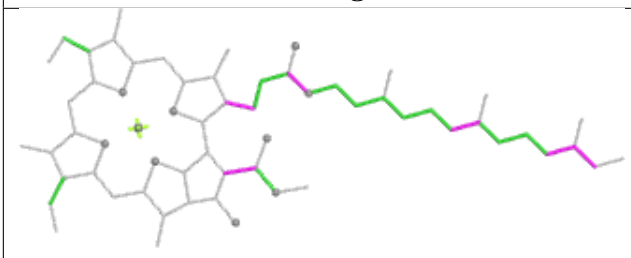
Ligand CLA c 608



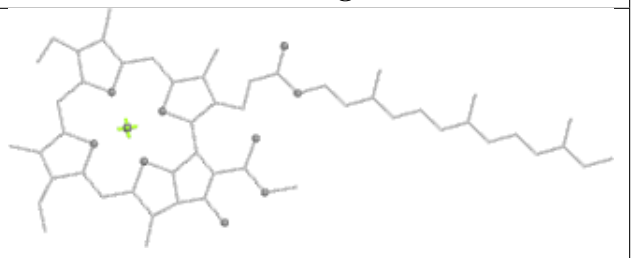
Bond lengths



Bond angles

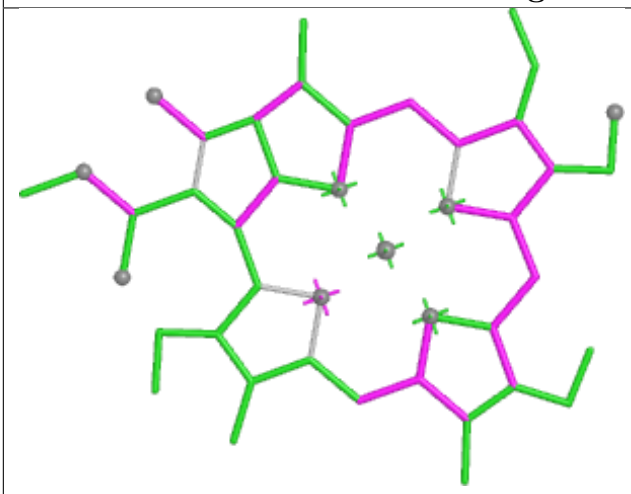


Torsions

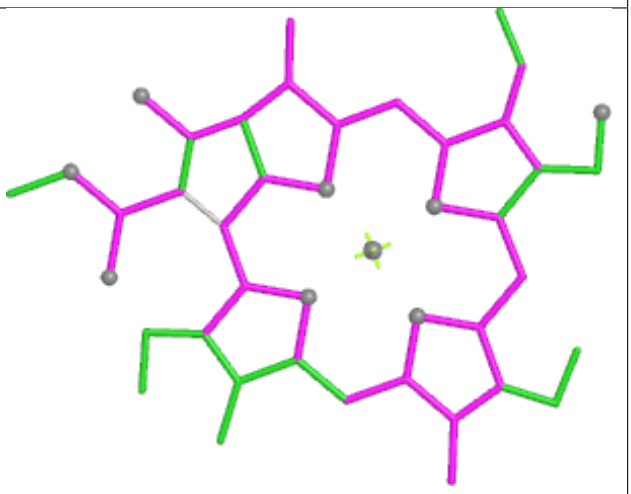


Rings

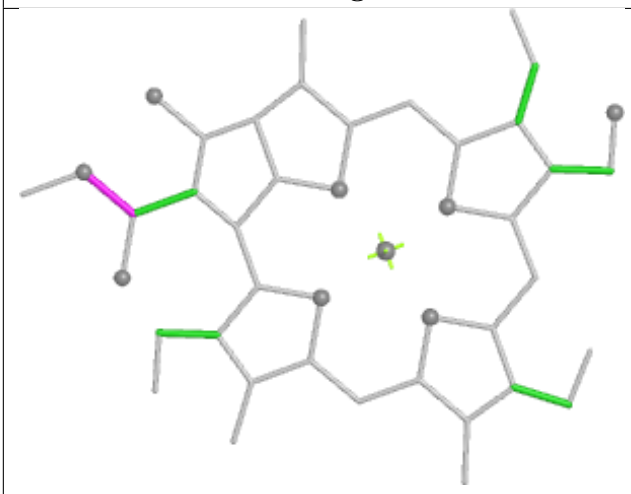
Ligand CHL 9 308



Bond lengths



Bond angles

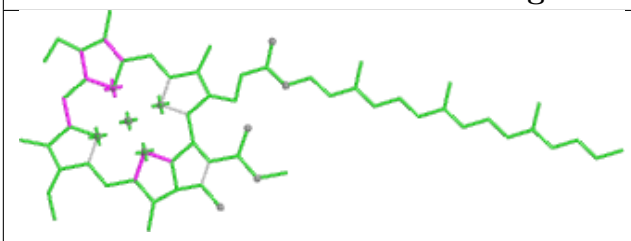


Torsions

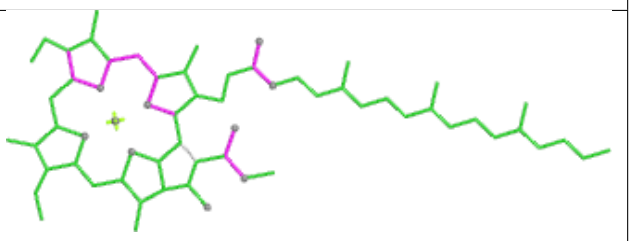


Rings

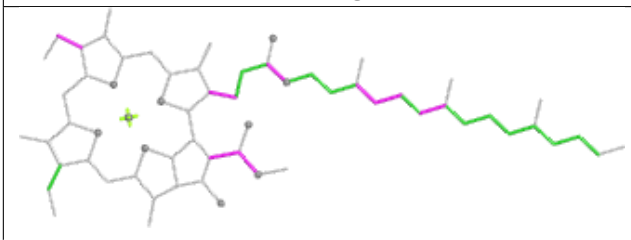
Ligand CLA u 315



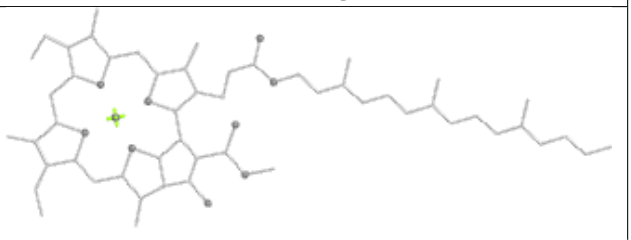
Bond lengths



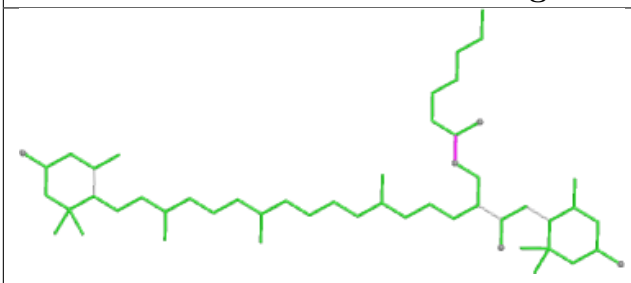
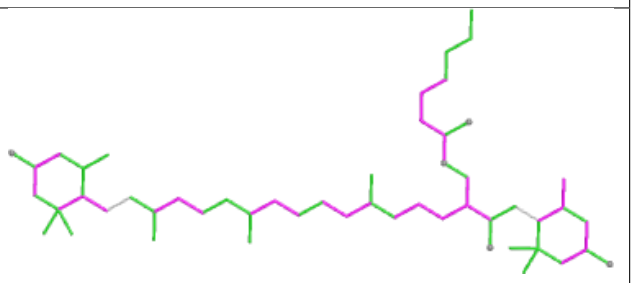
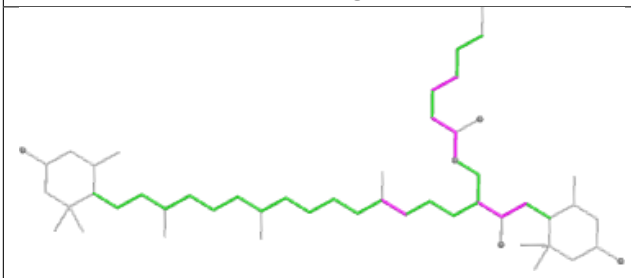
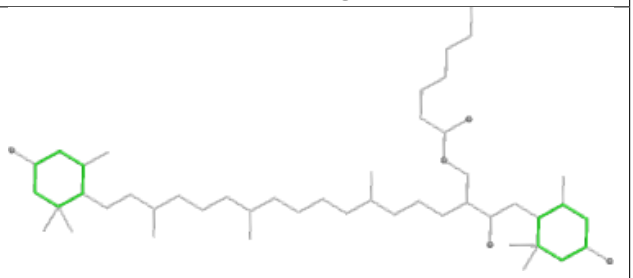
Bond angles

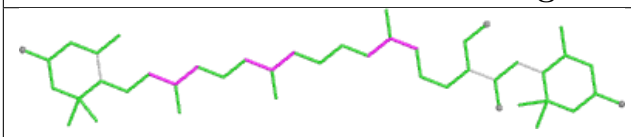
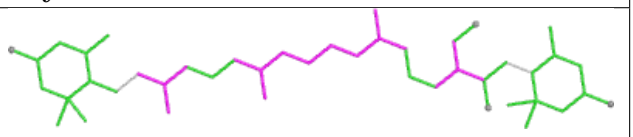
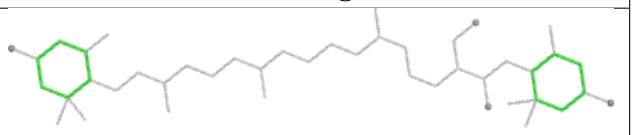


Torsions

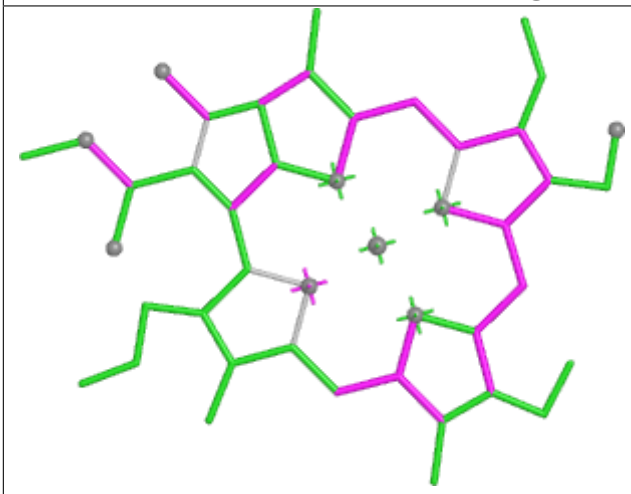


Rings

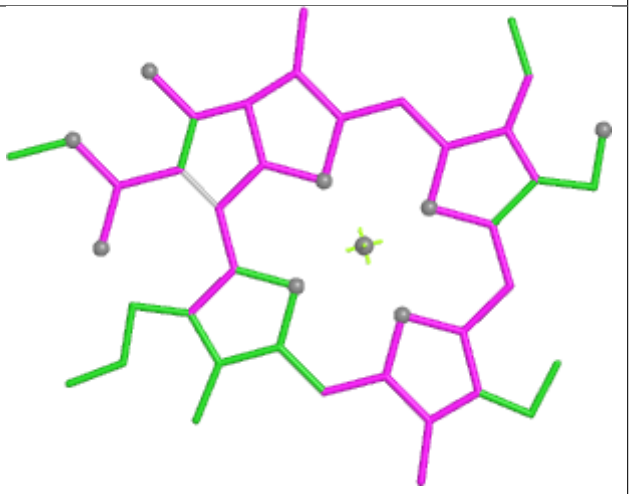
Ligand 0UR 9 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 0IE y 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

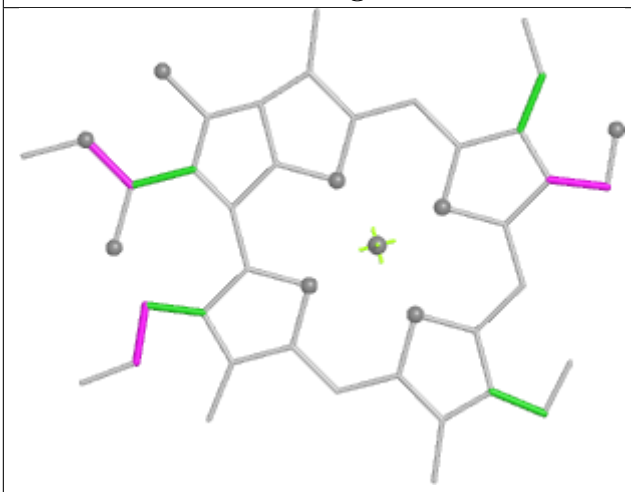
Ligand CHL 3 311



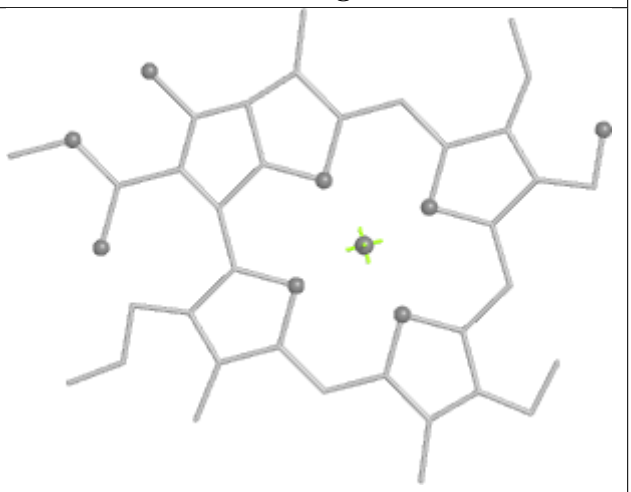
Bond lengths



Bond angles

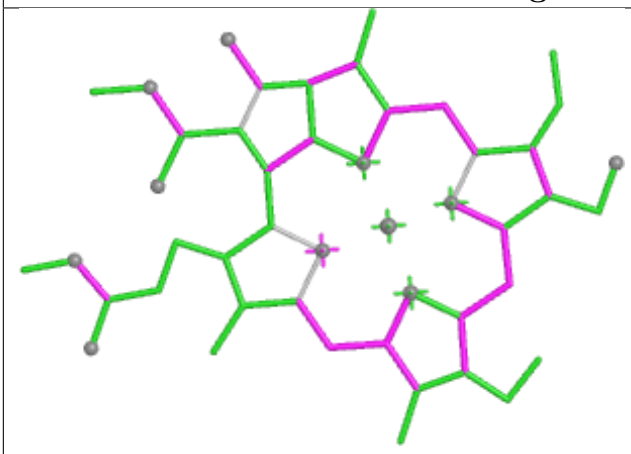


Torsions

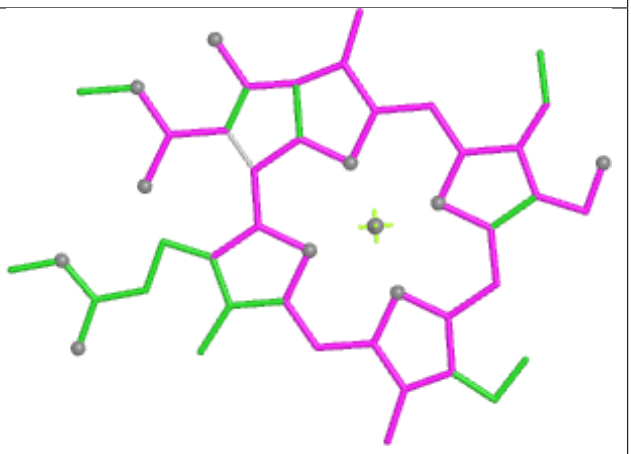


Rings

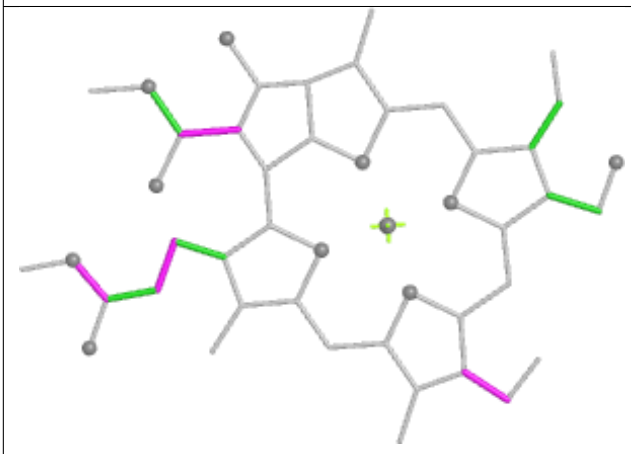
Ligand CHL r 303



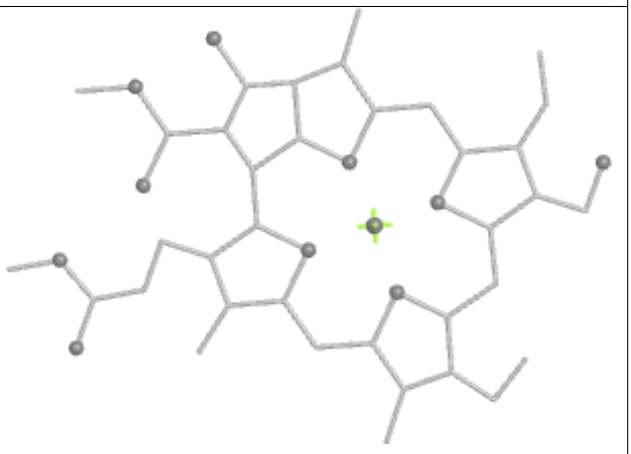
Bond lengths



Bond angles

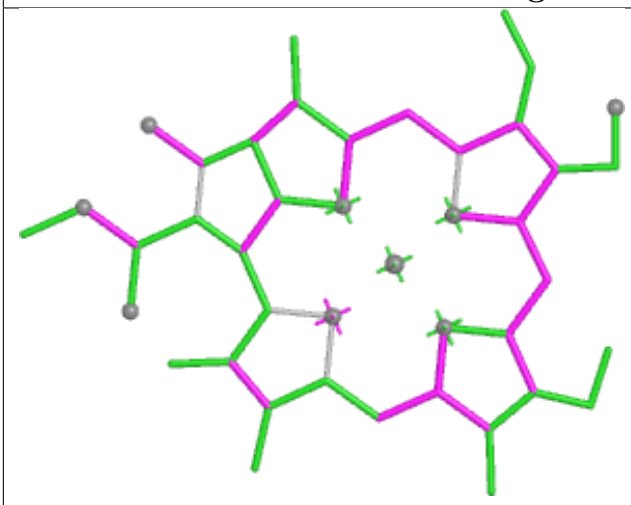


Torsions

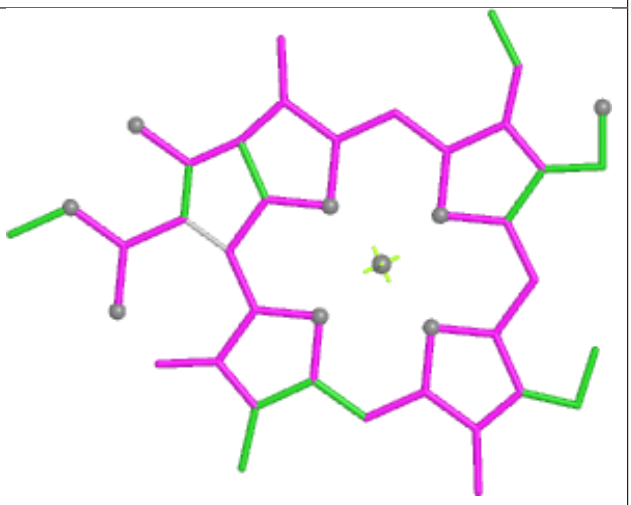


Rings

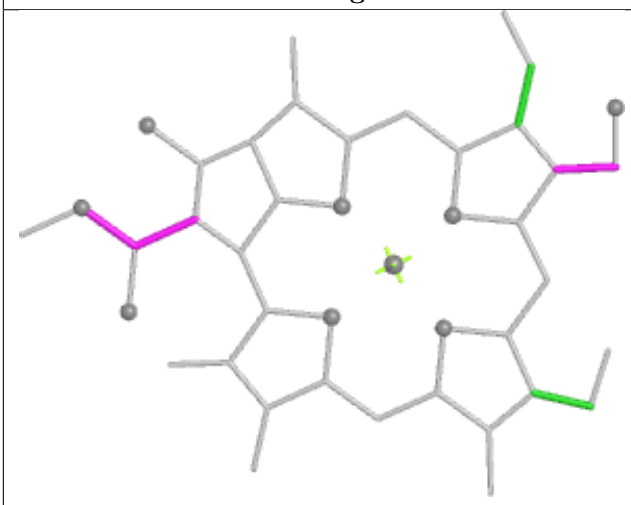
Ligand CHL 4 317



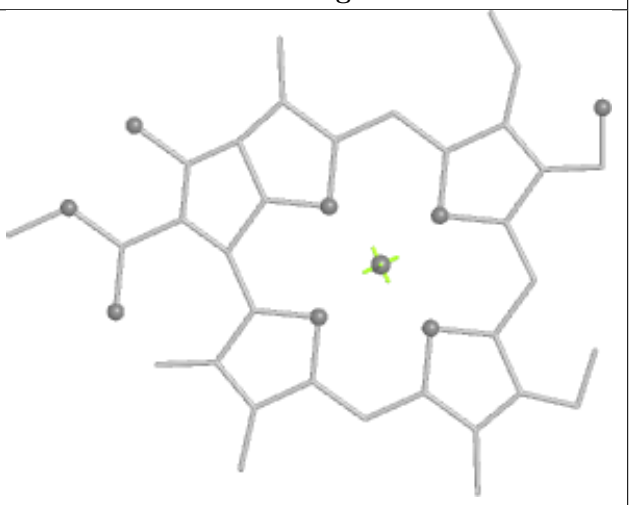
Bond lengths



Bond angles

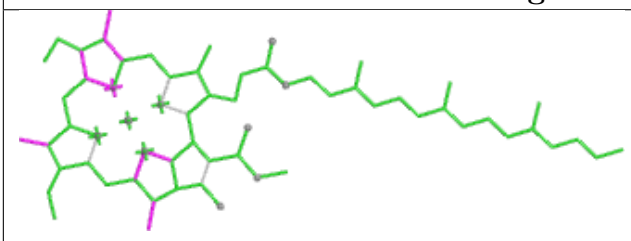


Torsions

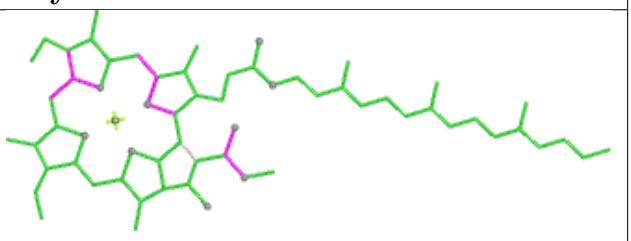


Rings

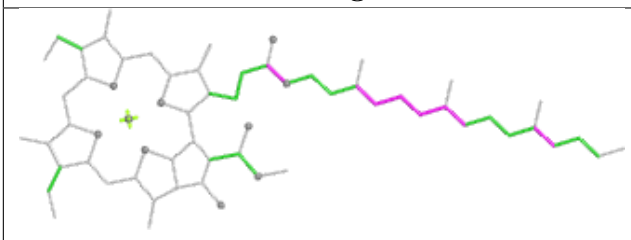
Ligand CLA y 315



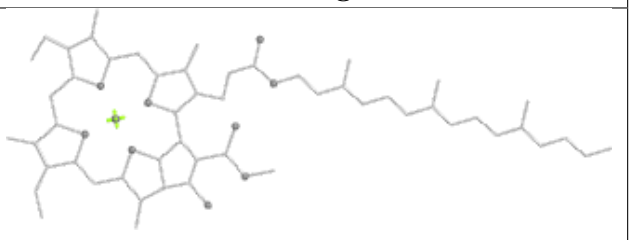
Bond lengths



Bond angles

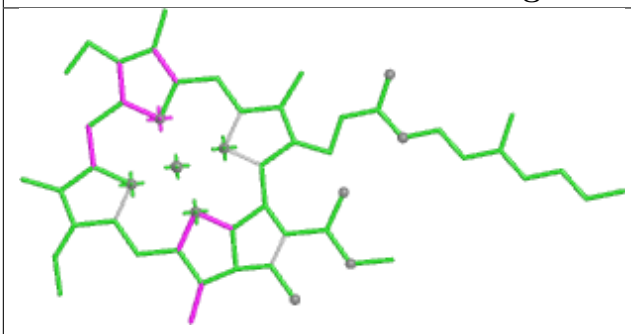


Torsions

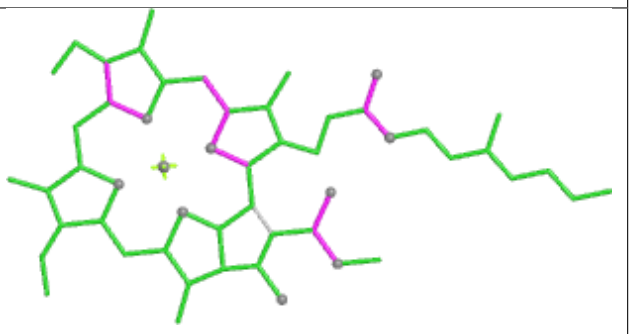


Rings

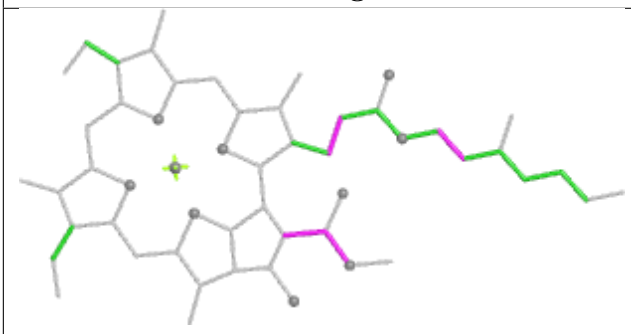
Ligand CLA G 307



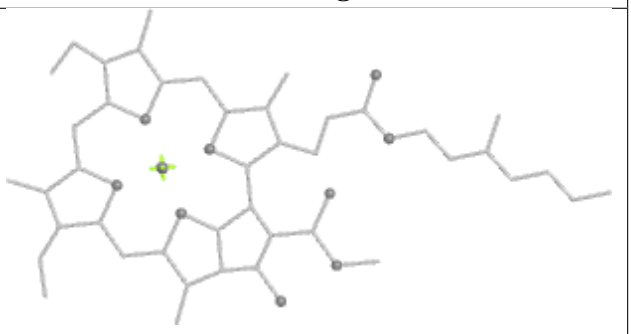
Bond lengths



Bond angles

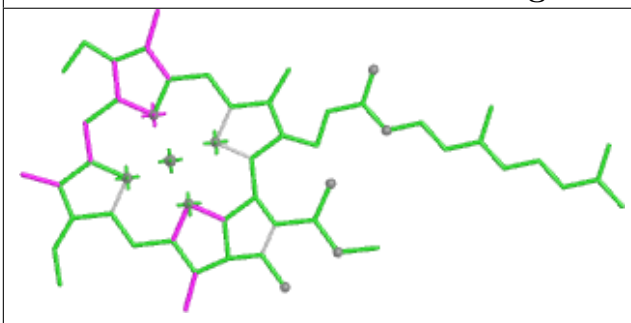


Torsions

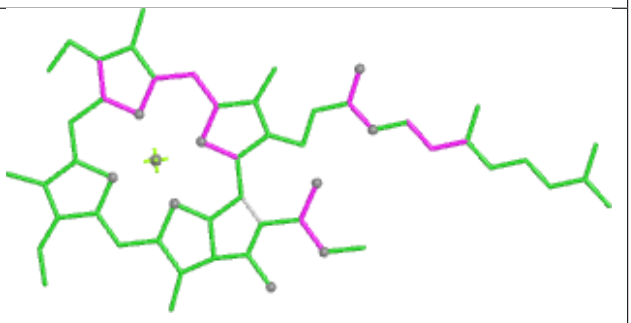


Rings

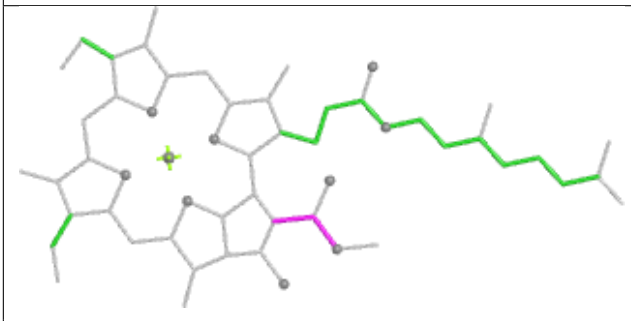
Ligand CLA 8 311



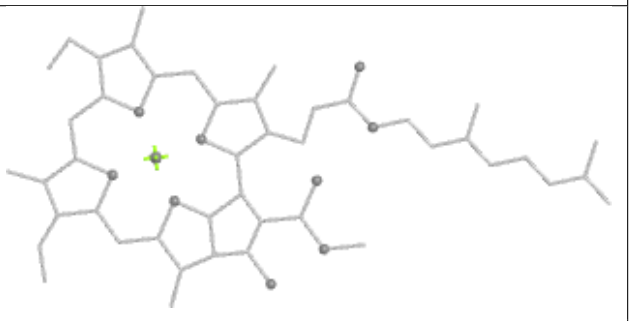
Bond lengths



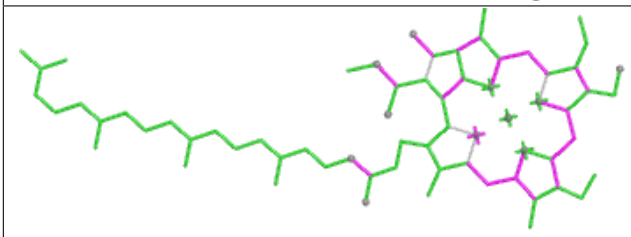
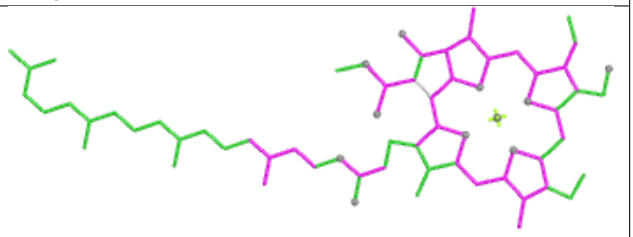
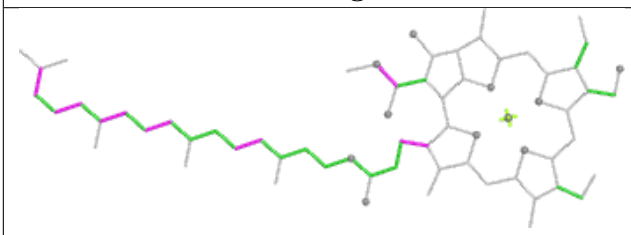
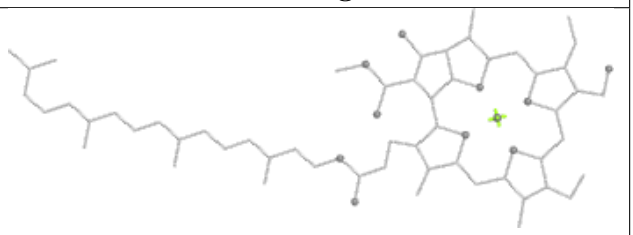
Bond angles

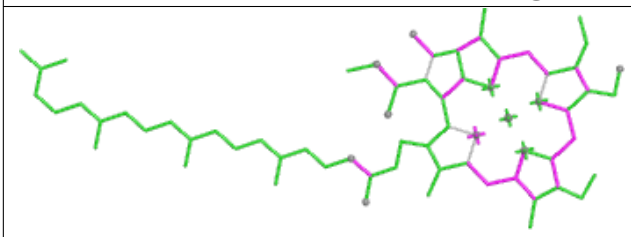
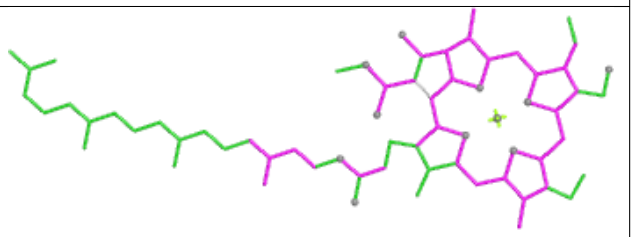
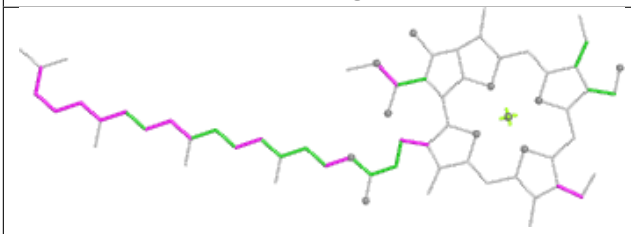
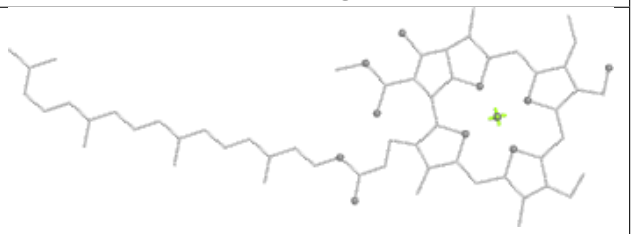


Torsions

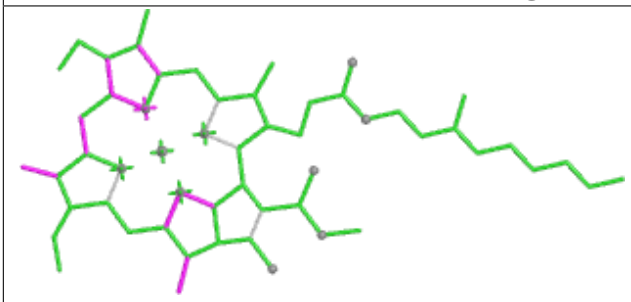


Rings

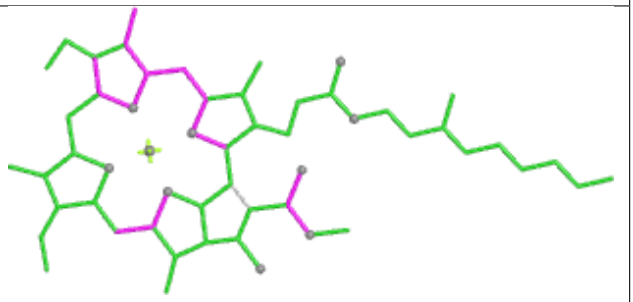
Ligand CHL y 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 7 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

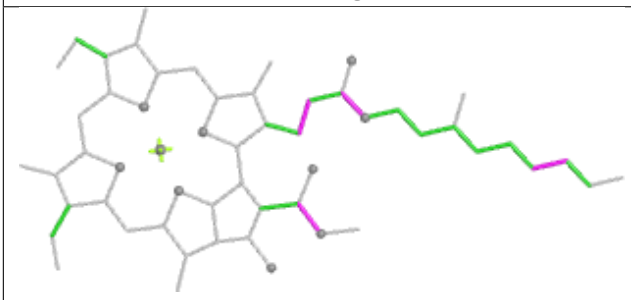
Ligand CLA G 317



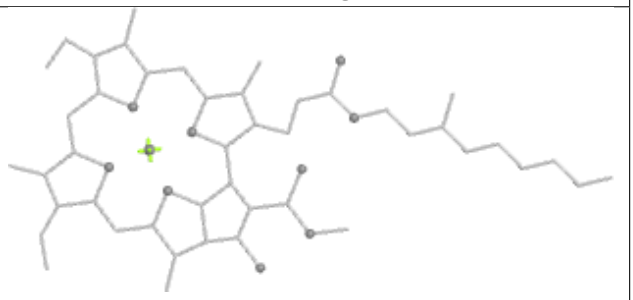
Bond lengths



Bond angles

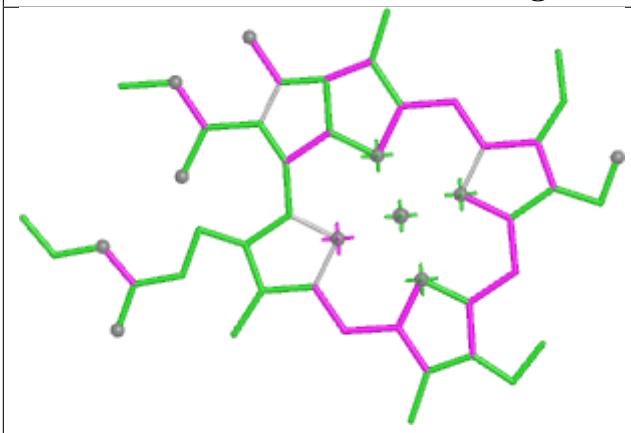


Torsions

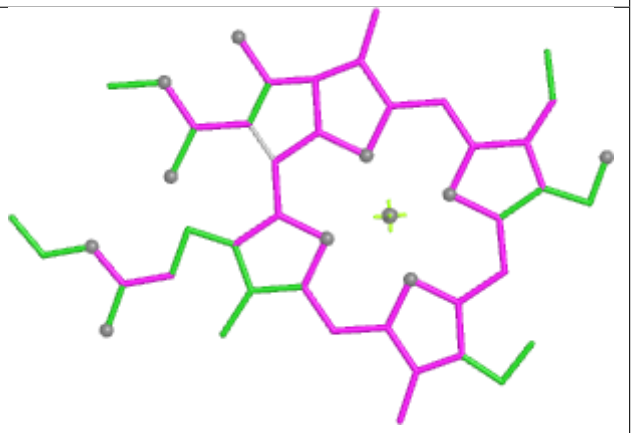


Rings

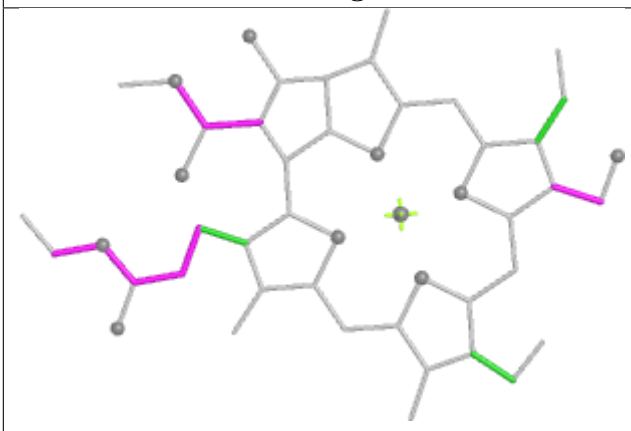
Ligand CHL r 308



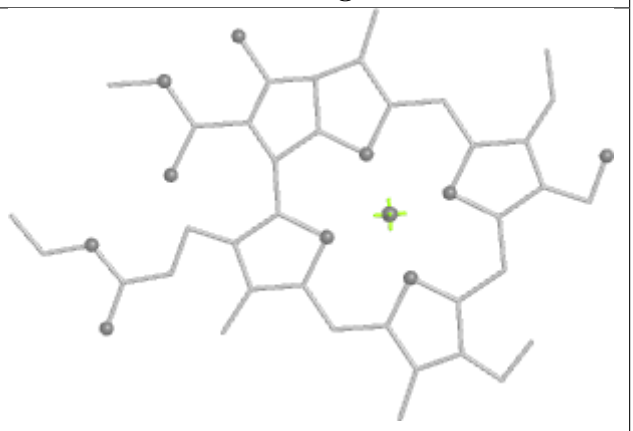
Bond lengths



Bond angles

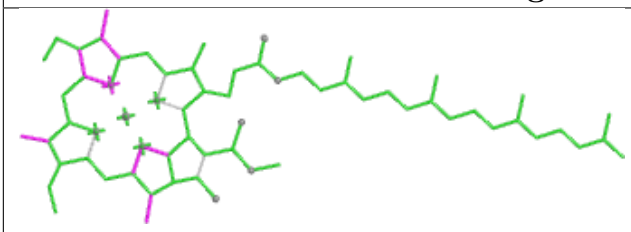


Torsions

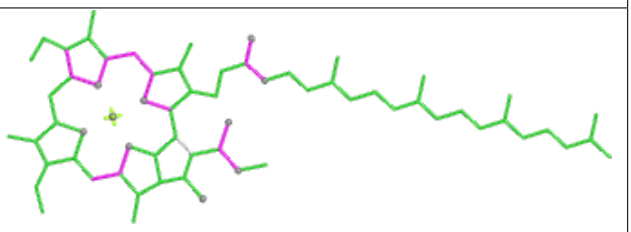


Rings

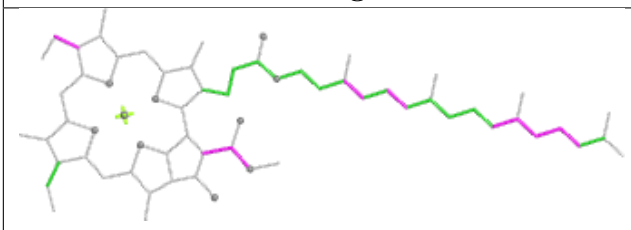
Ligand CLA b 605



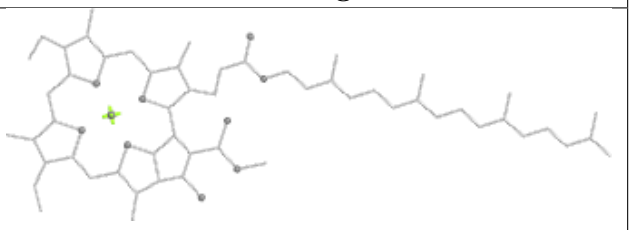
Bond lengths



Bond angles

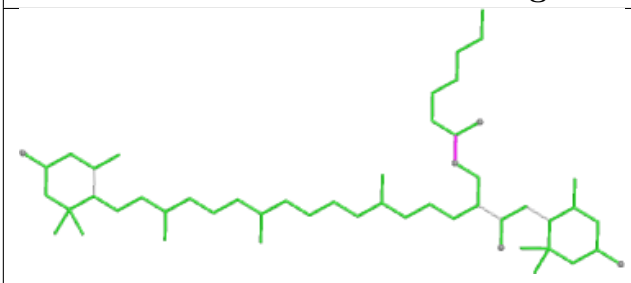


Torsions

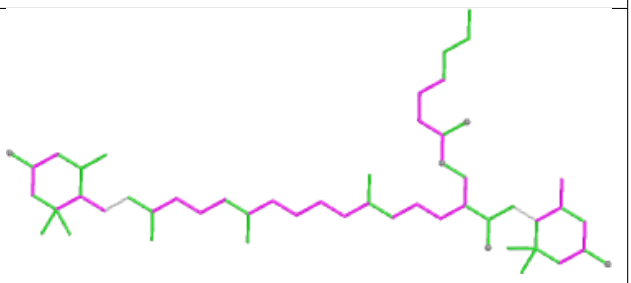


Rings

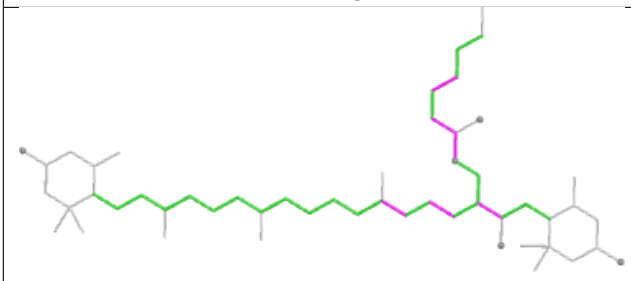
Ligand 0UR 6 301



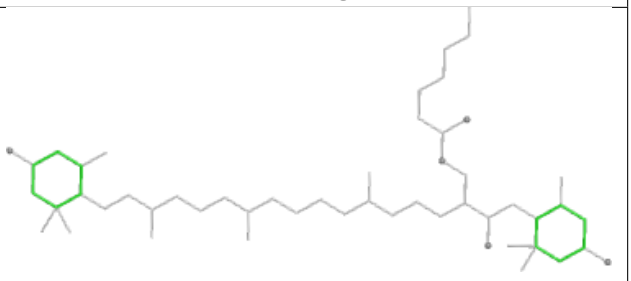
Bond lengths



Bond angles

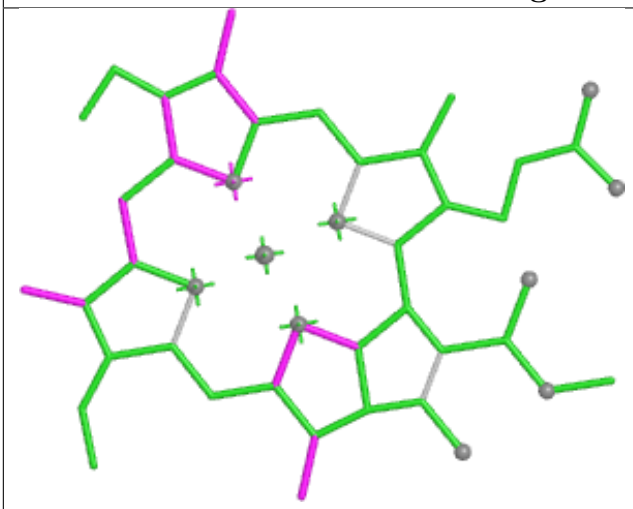


Torsions

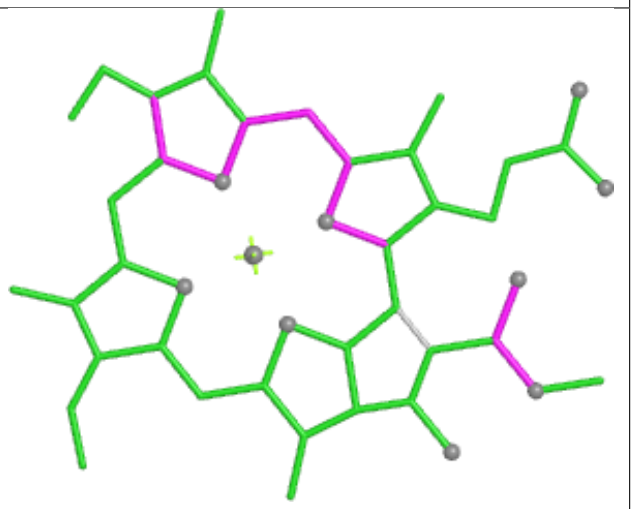


Rings

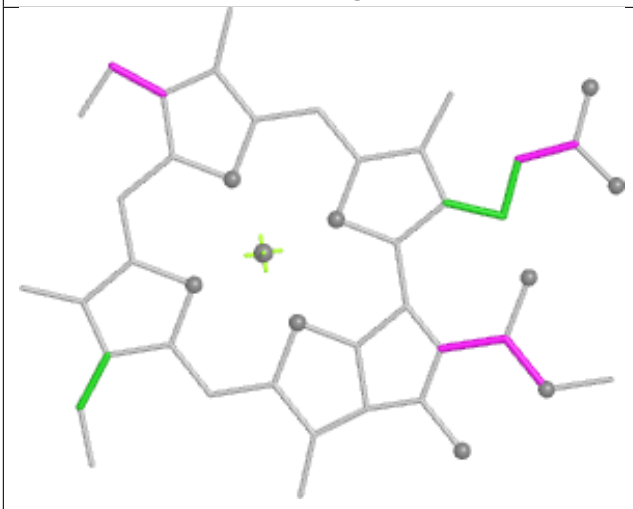
Ligand CLA r 312



Bond lengths



Bond angles

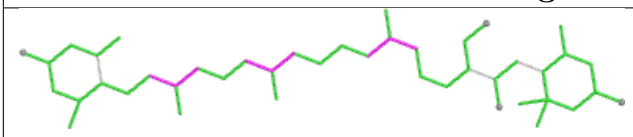


Torsions

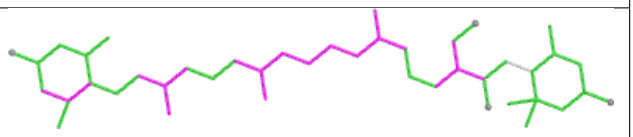


Rings

Ligand 0IE 3 302



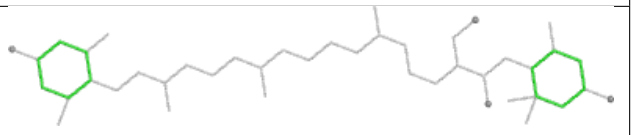
Bond lengths



Bond angles

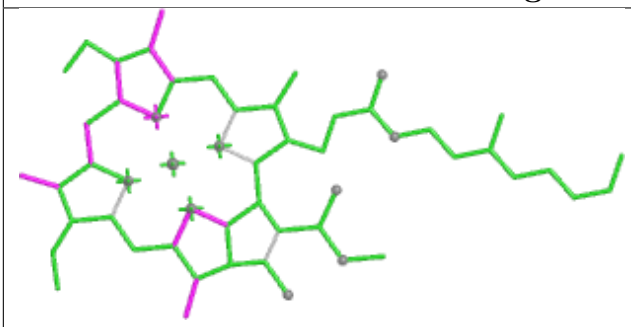


Torsions

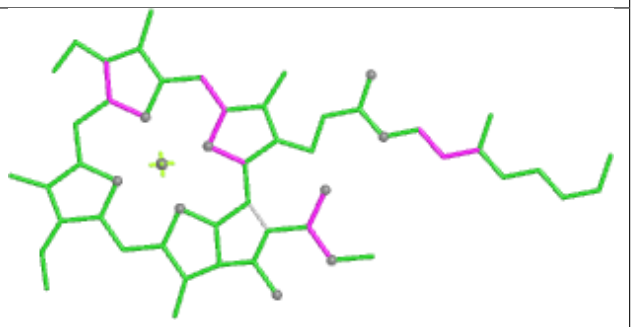


Rings

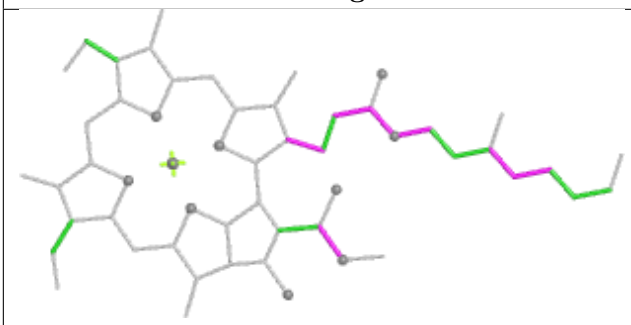
Ligand CLA C 612



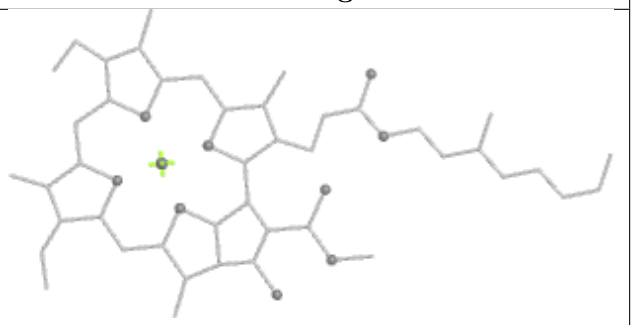
Bond lengths



Bond angles

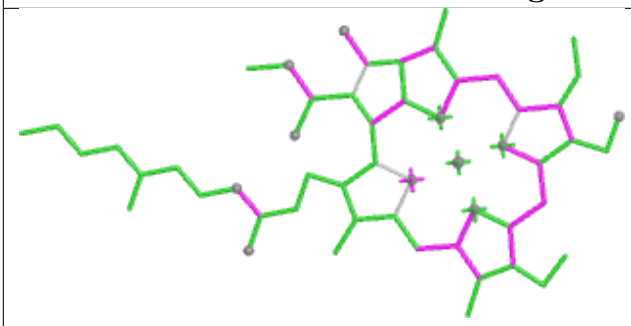


Torsions

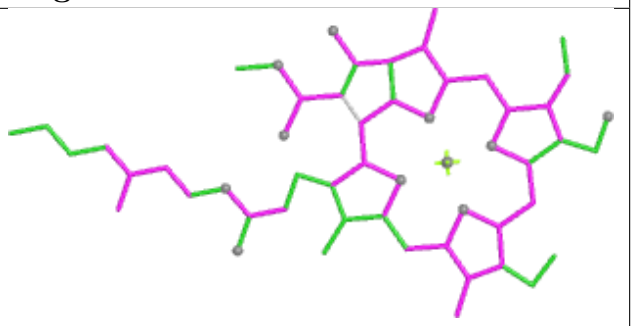


Rings

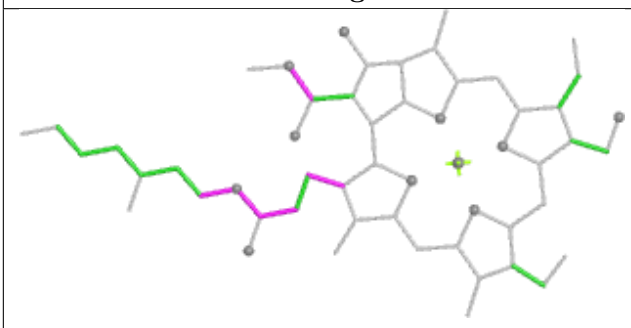
Ligand CHL g 311



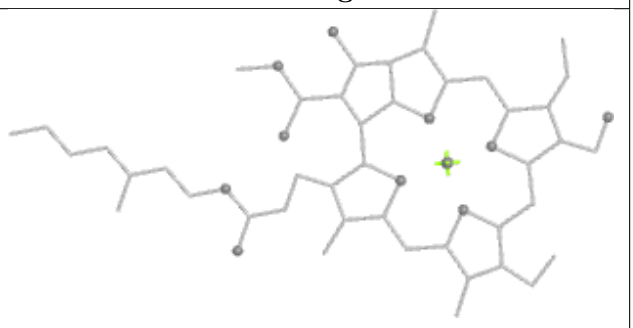
Bond lengths



Bond angles

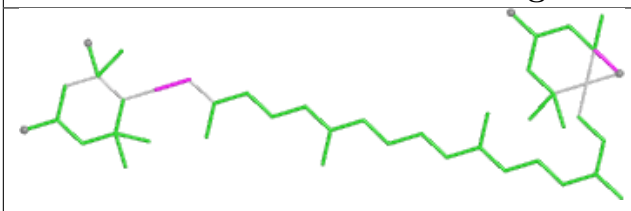


Torsions

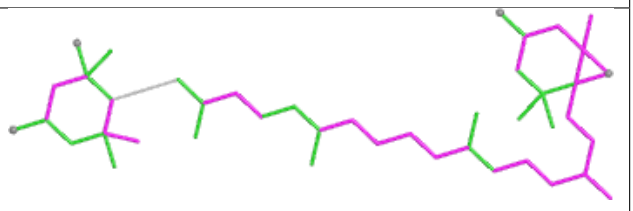


Rings

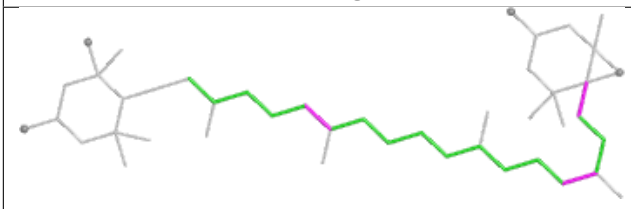
Ligand NEX s 401



Bond lengths



Bond angles

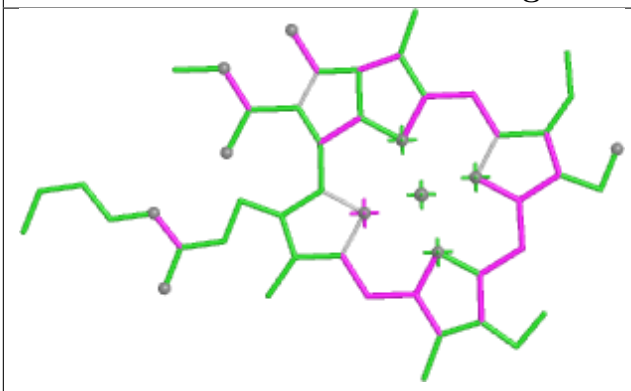


Torsions

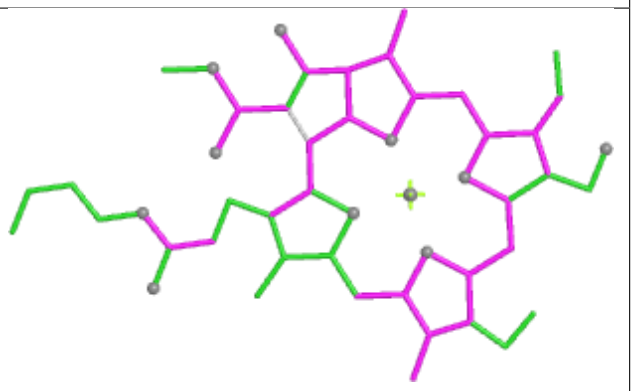


Rings

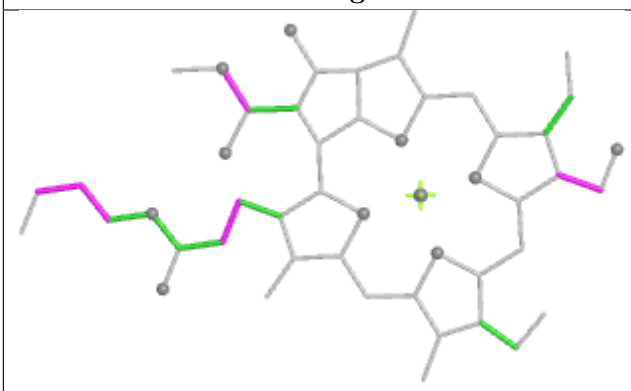
Ligand CHL N 311



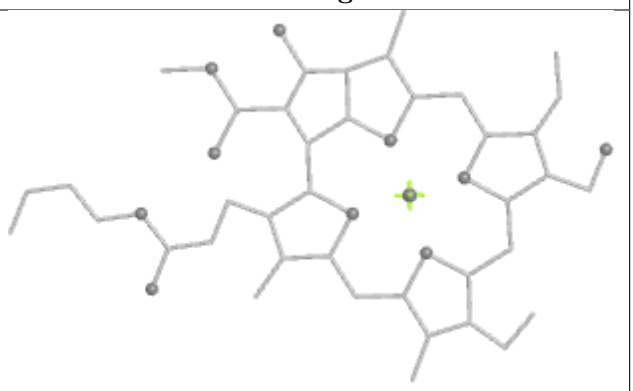
Bond lengths



Bond angles

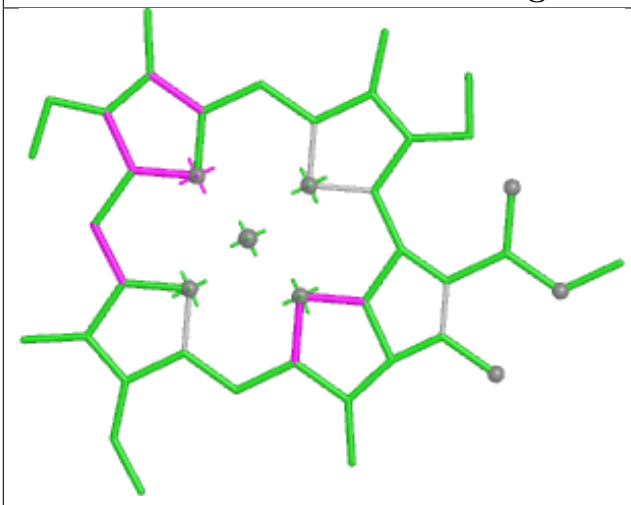


Torsions

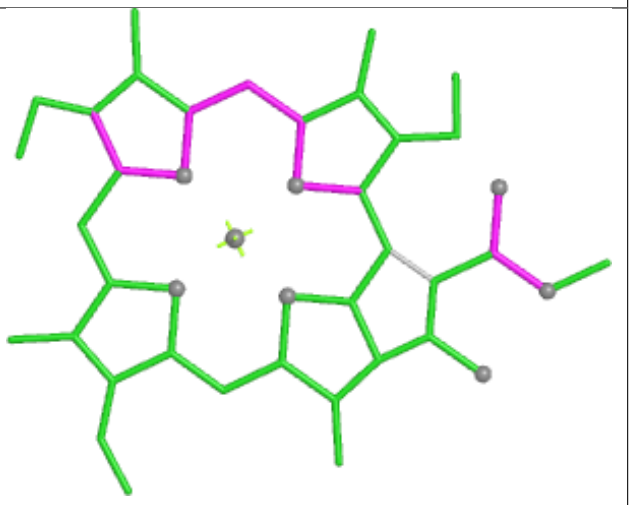


Rings

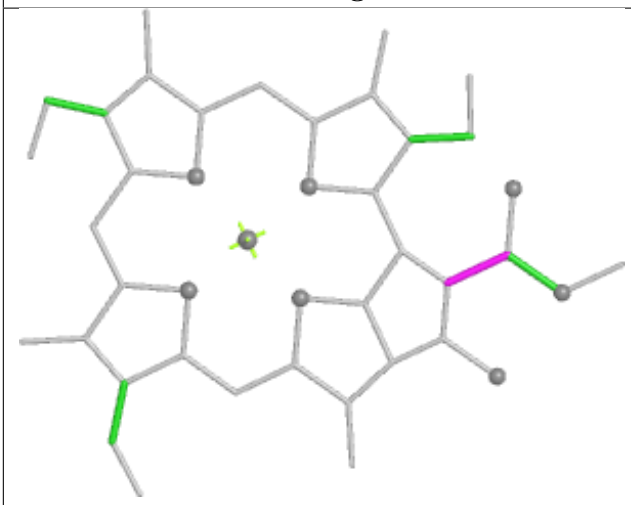
Ligand CLA 1 316



Bond lengths



Bond angles

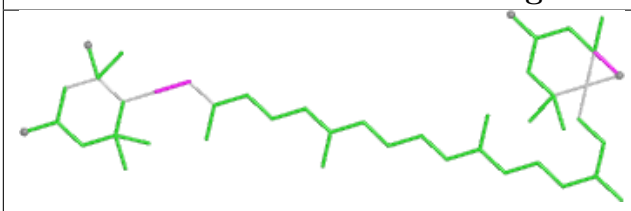


Torsions

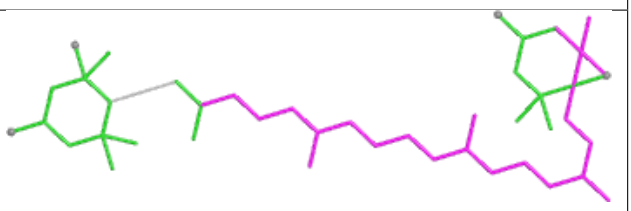


Rings

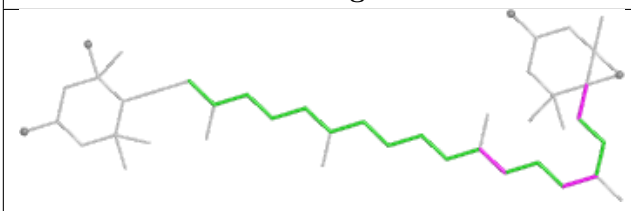
Ligand NEX u 304



Bond lengths



Bond angles

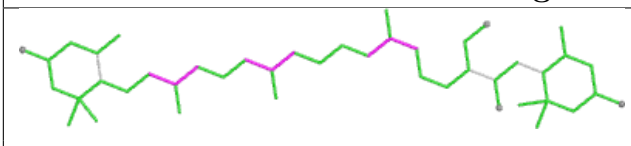


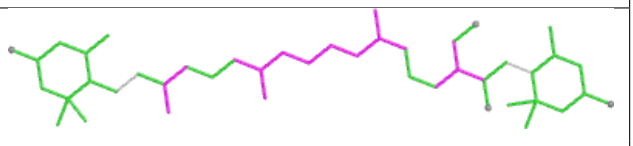
Torsions



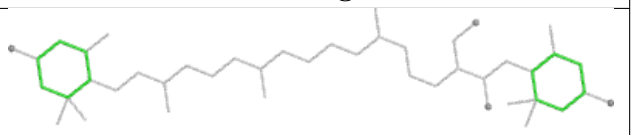
Rings

Ligand 0IE G 302

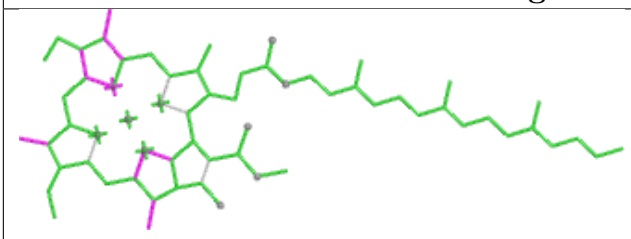

Bond lengths

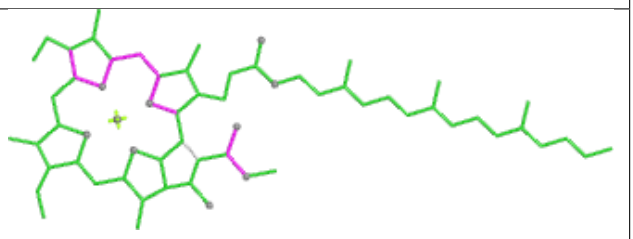

Bond angles

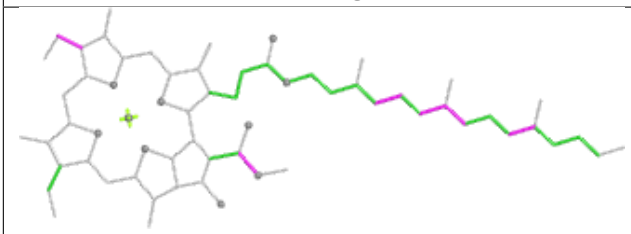

Torsions

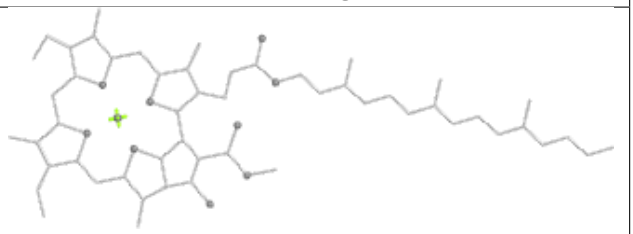

Rings

Ligand CLA 5 315

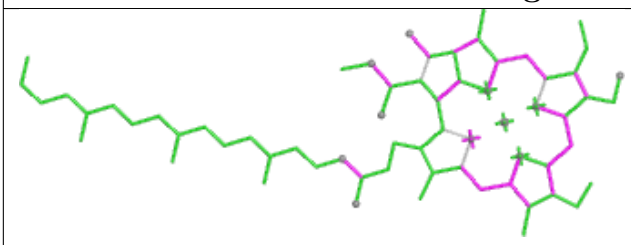

Bond lengths

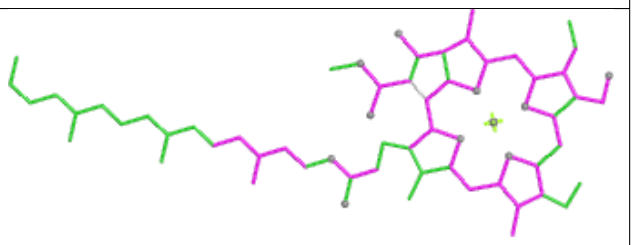

Bond angles

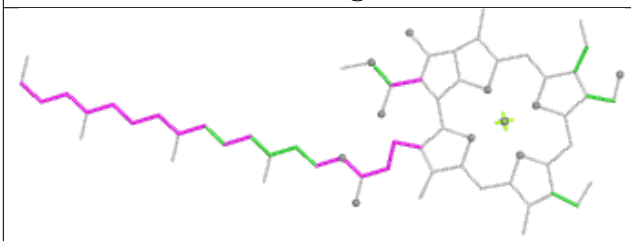

Torsions

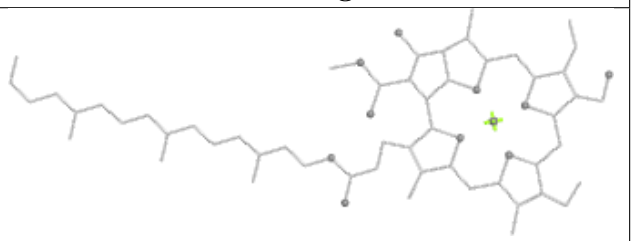

Rings

Ligand CHL Y 305

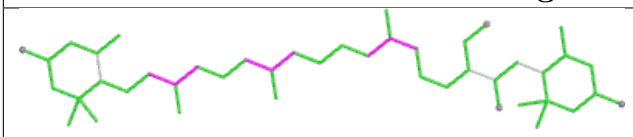

Bond lengths


Bond angles

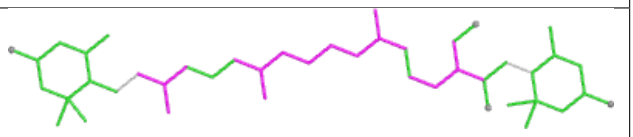

Torsions


Rings

Ligand 0IE u 302



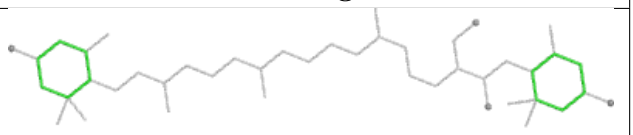
Bond lengths



Bond angles

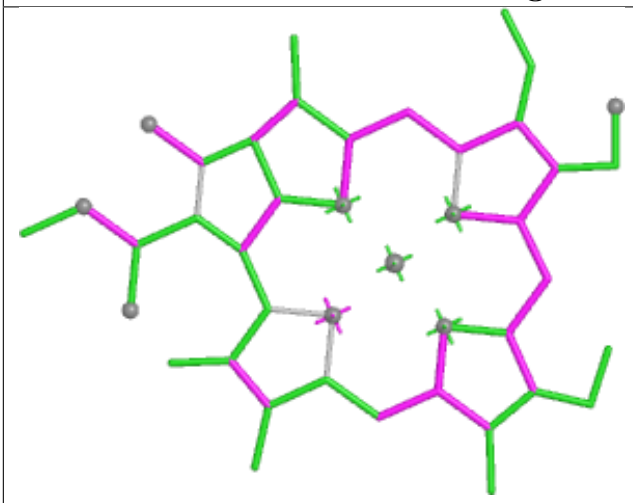


Torsions

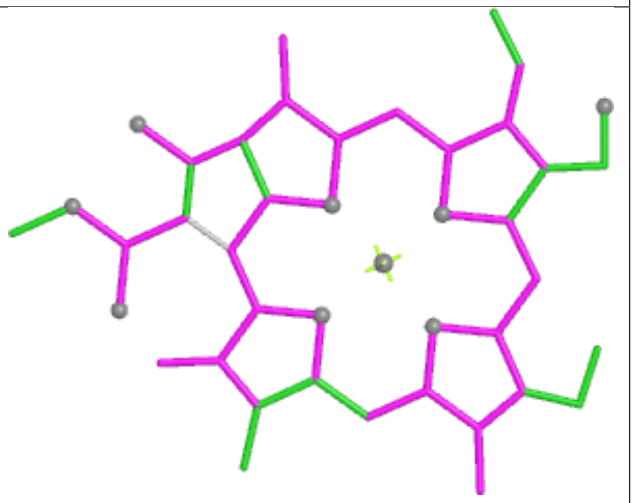


Rings

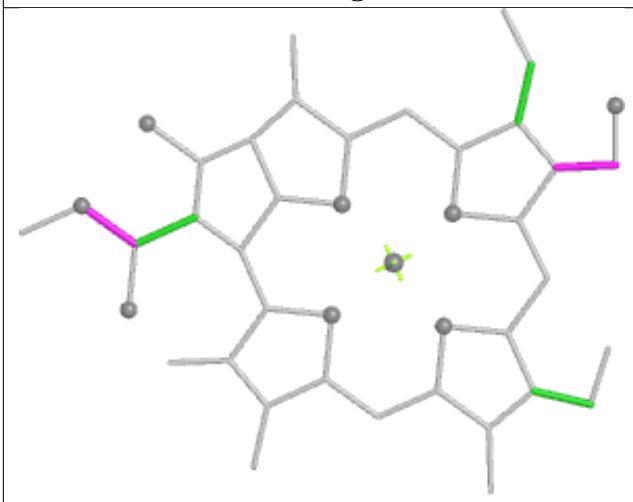
Ligand CHL n 317



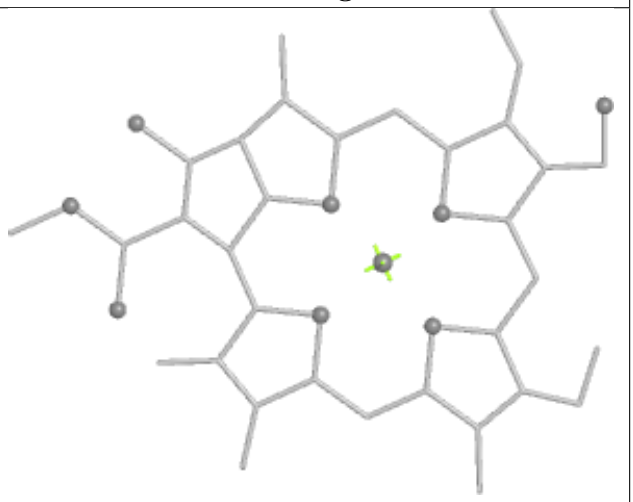
Bond lengths



Bond angles

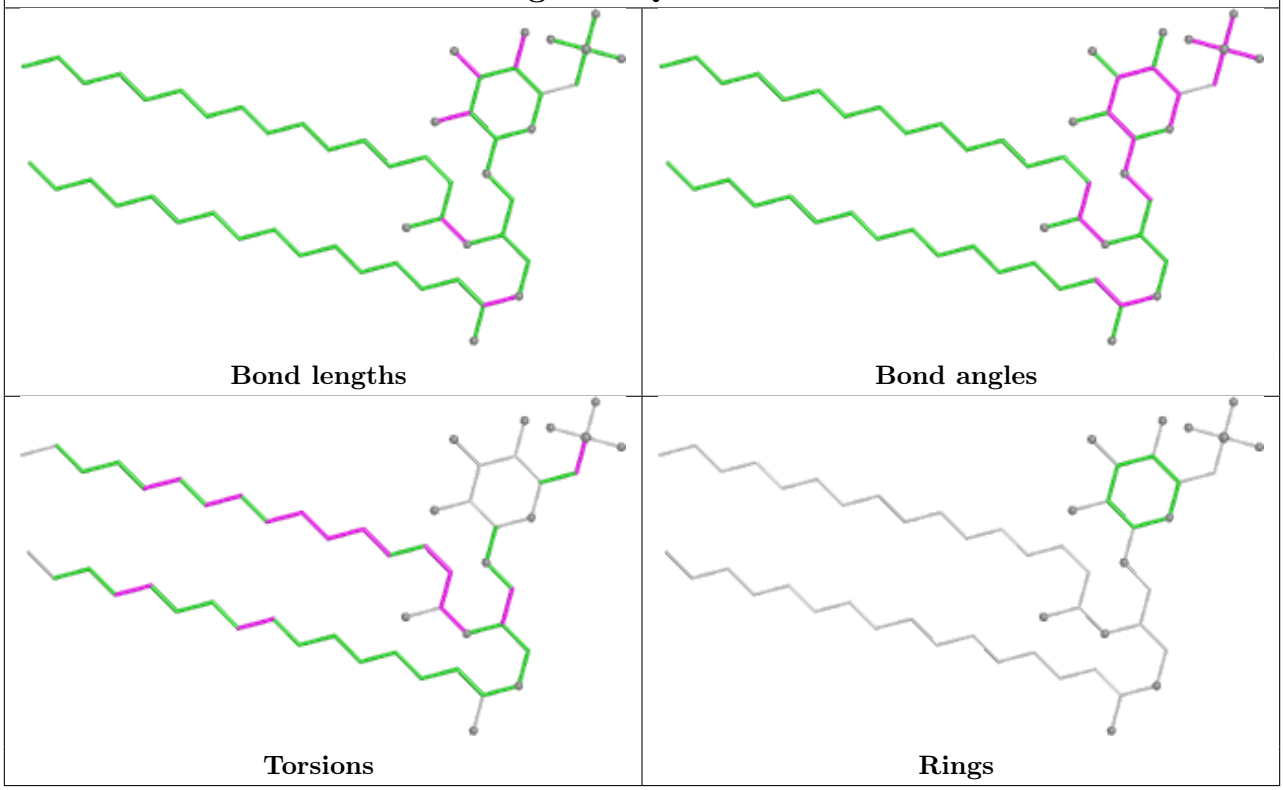


Torsions

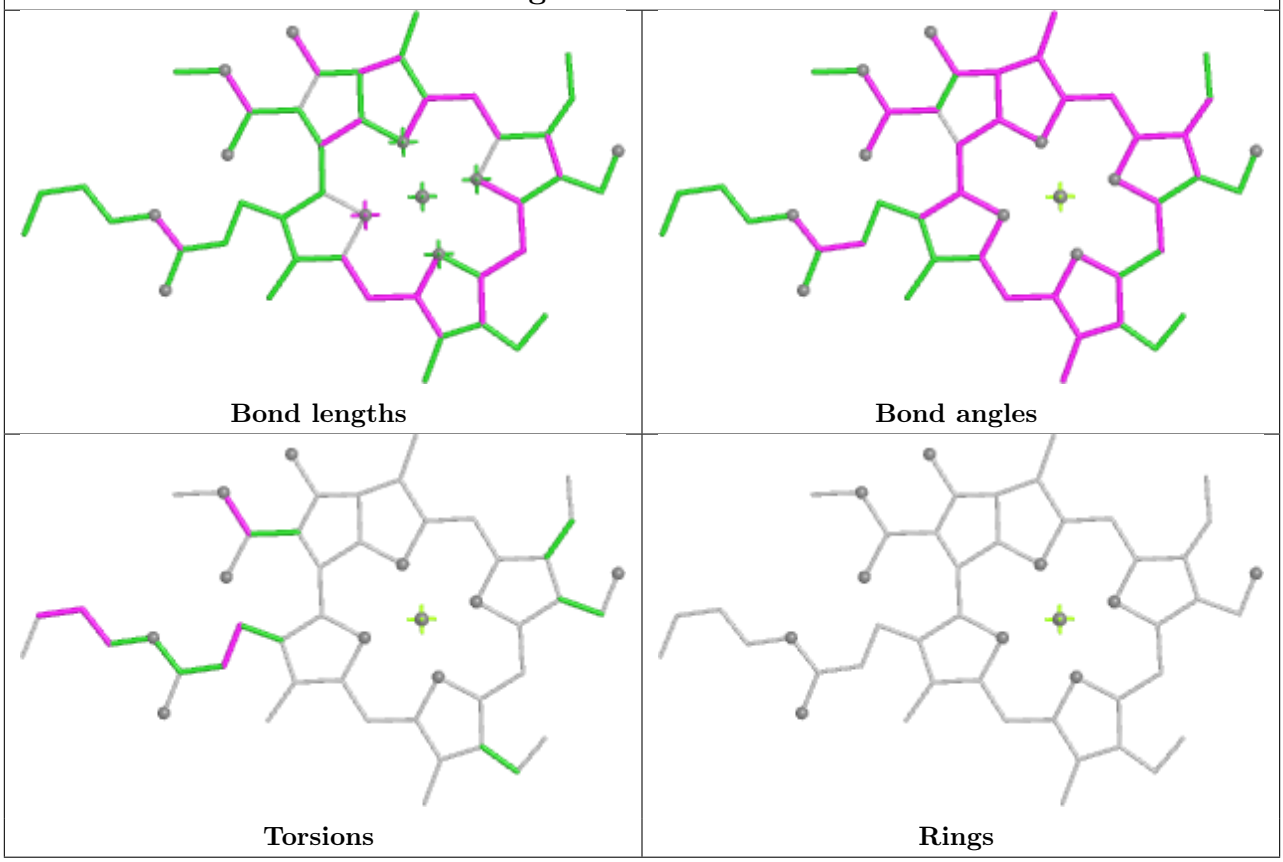


Rings

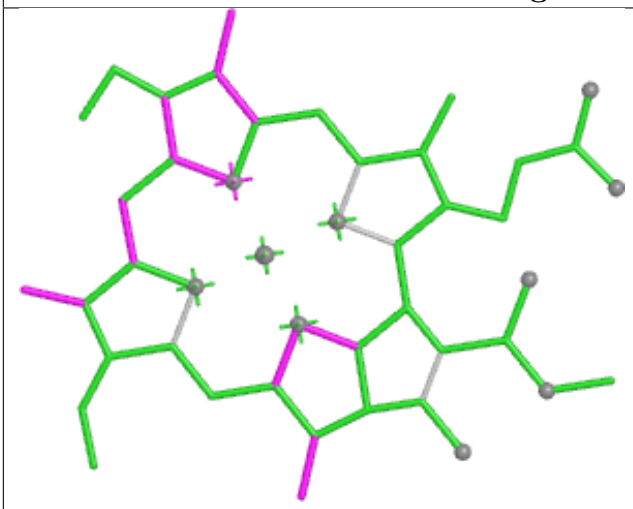
Ligand SQD b 618



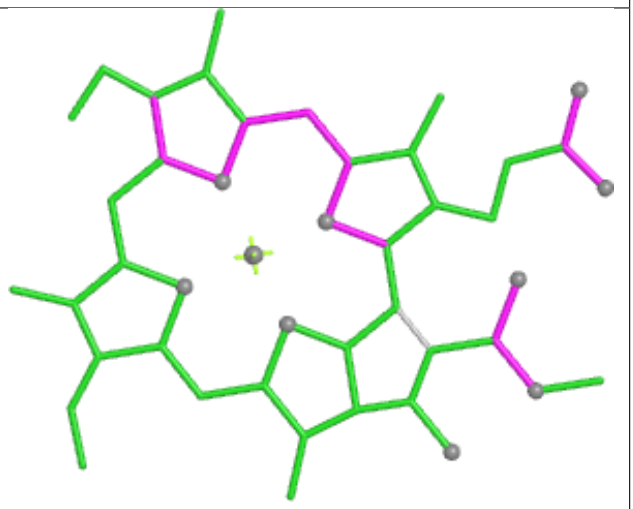
Ligand CHL 8 309



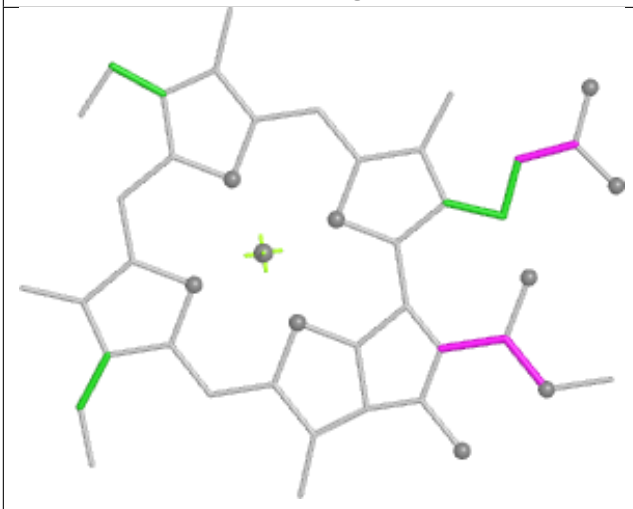
Ligand CLA s 412



Bond lengths



Bond angles

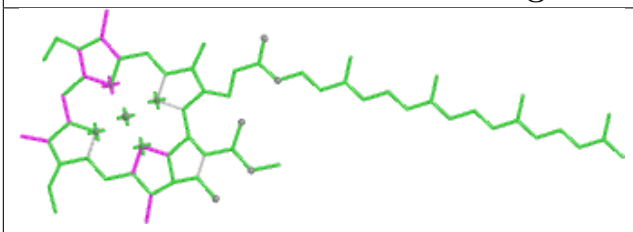


Torsions

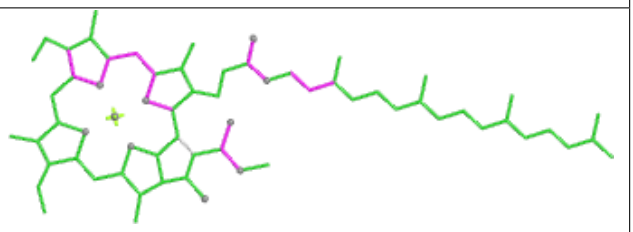


Rings

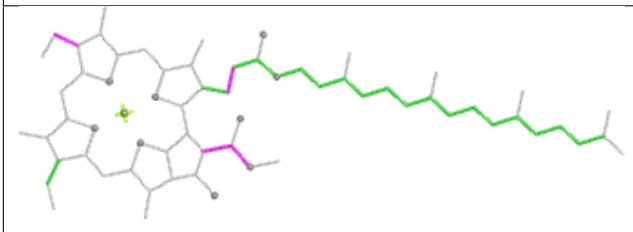
Ligand CLA b 610



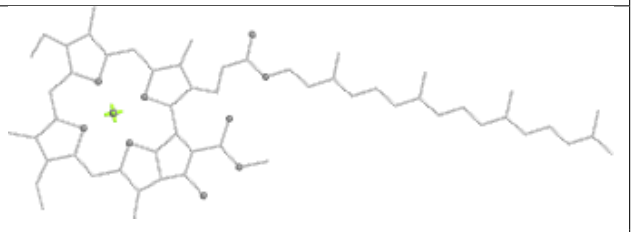
Bond lengths



Bond angles

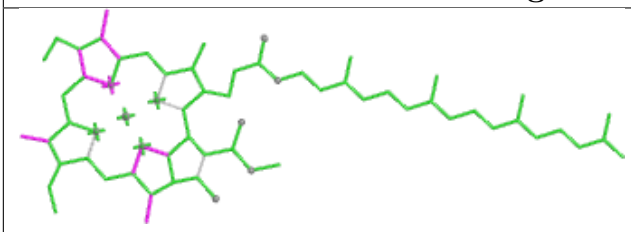


Torsions

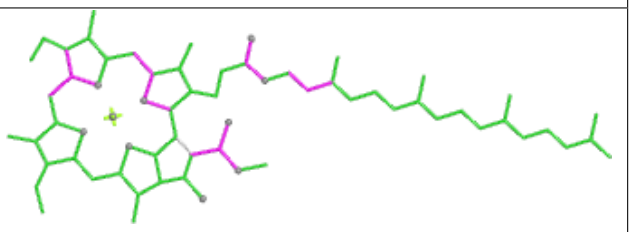


Rings

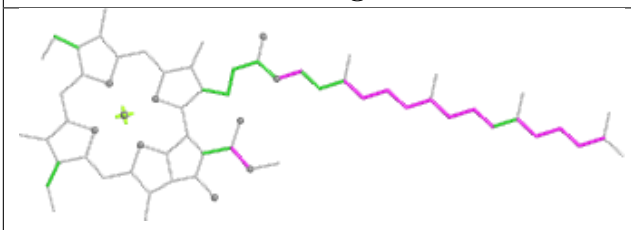
Ligand CLA b 609



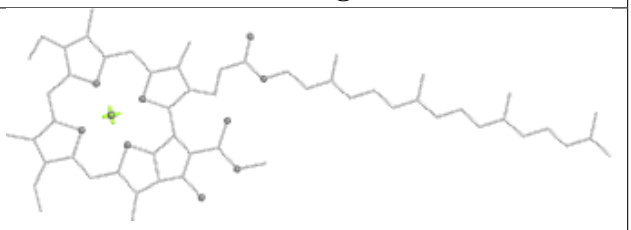
Bond lengths



Bond angles



Torsions

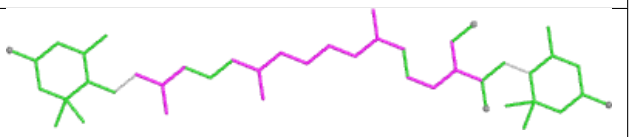


Rings

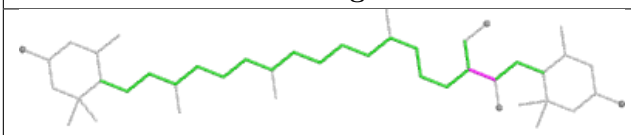
Ligand 0IE n 302



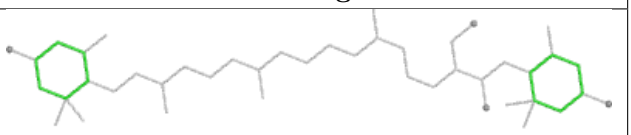
Bond lengths



Bond angles

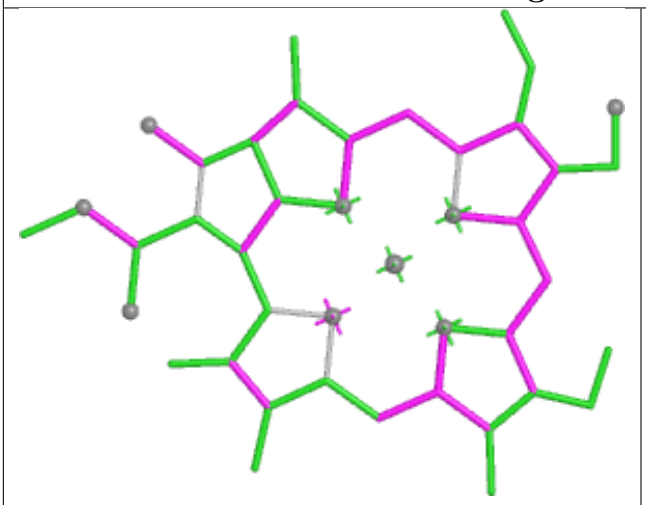


Torsions

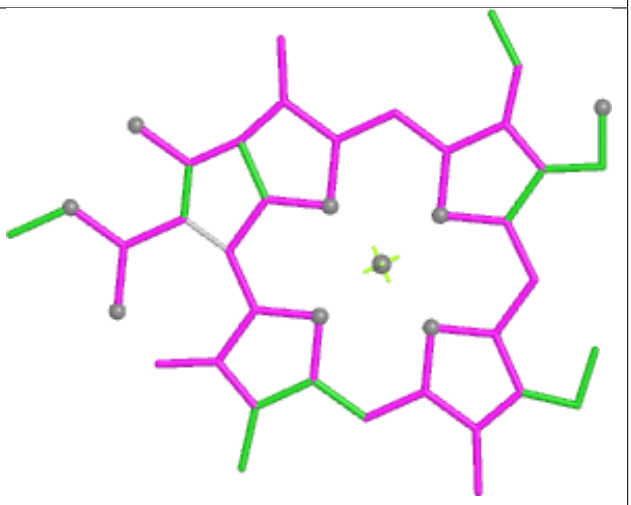


Rings

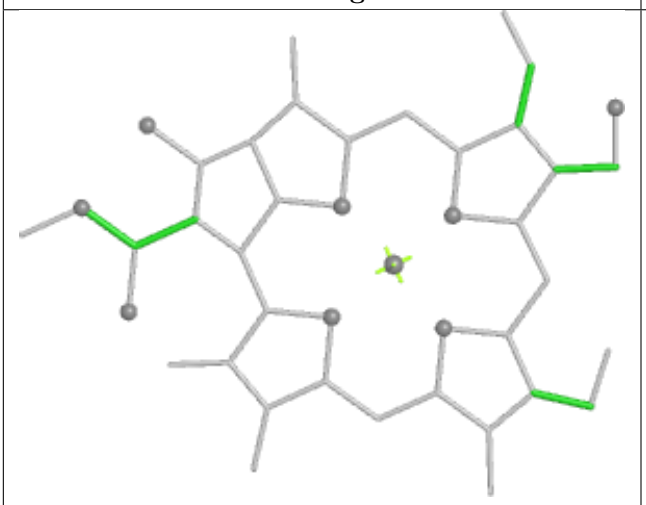
Ligand CHL 8 315



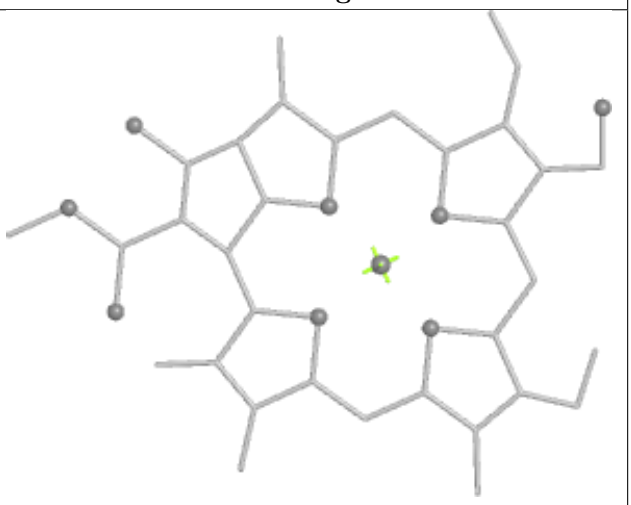
Bond lengths



Bond angles

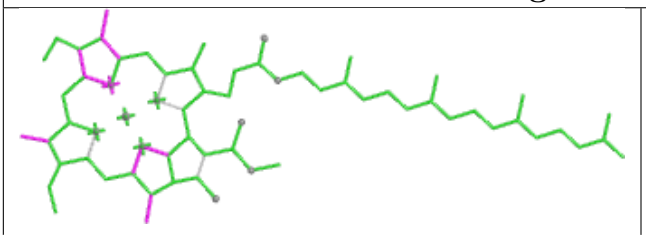


Torsions

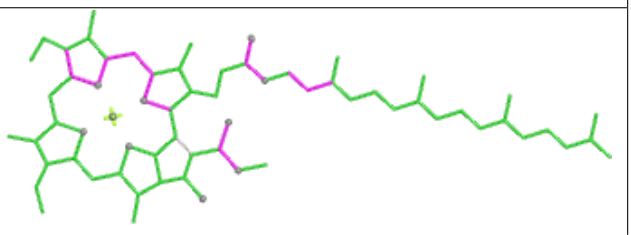


Rings

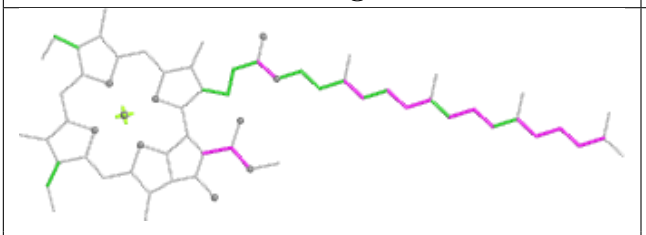
Ligand CLA c 604



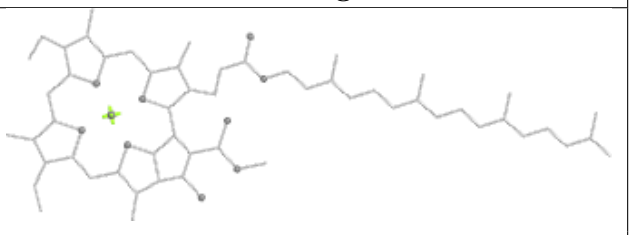
Bond lengths



Bond angles

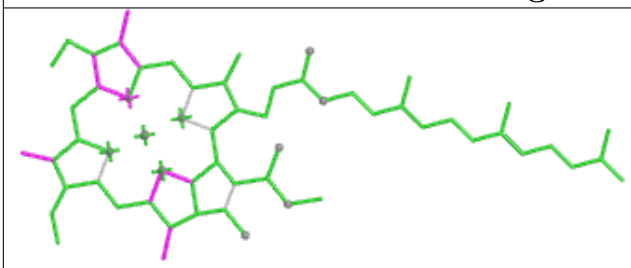


Torsions

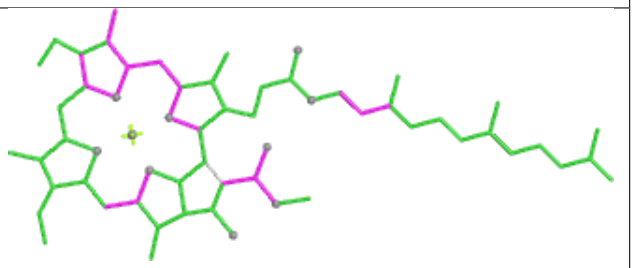


Rings

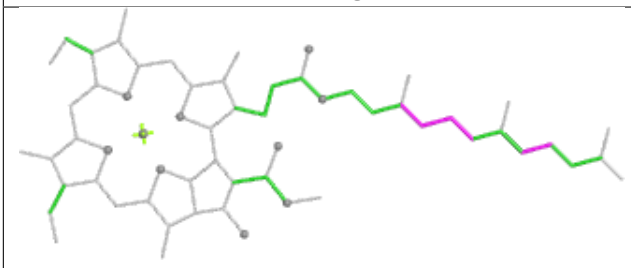
Ligand CLA a 607



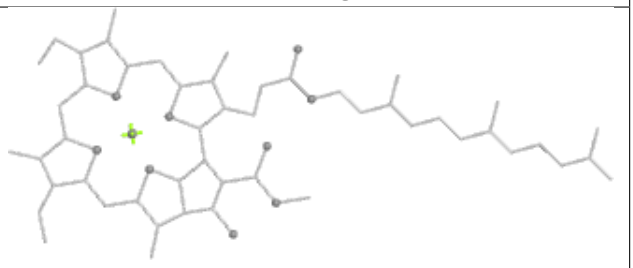
Bond lengths



Bond angles

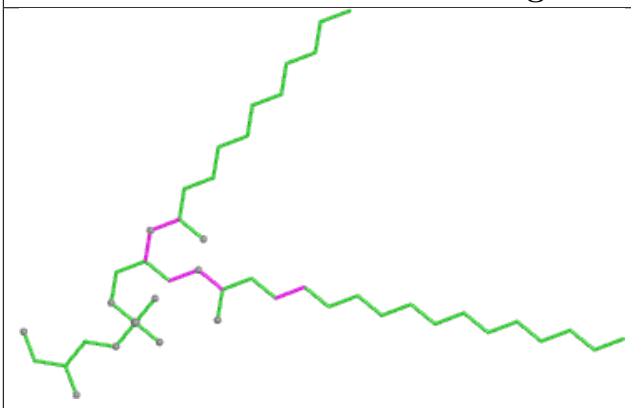


Torsions

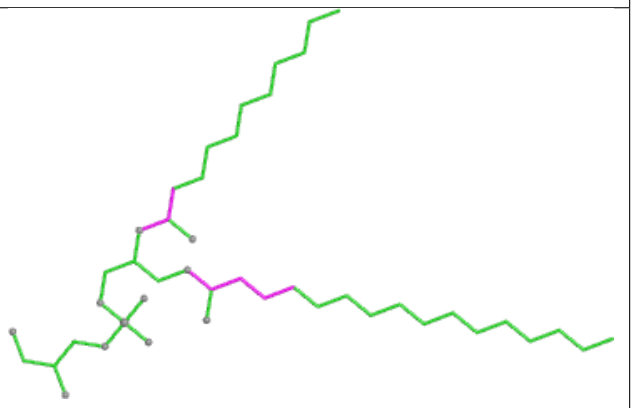


Rings

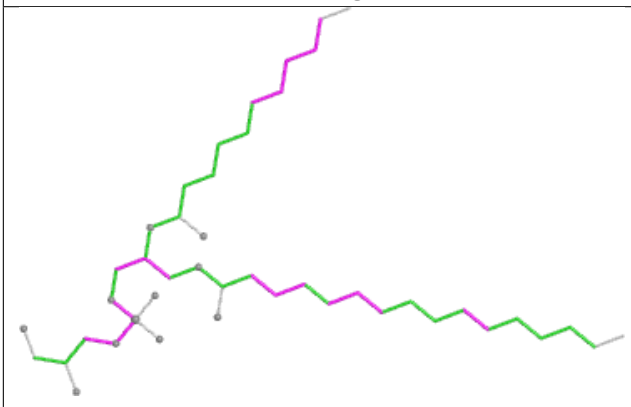
Ligand LHG a 612



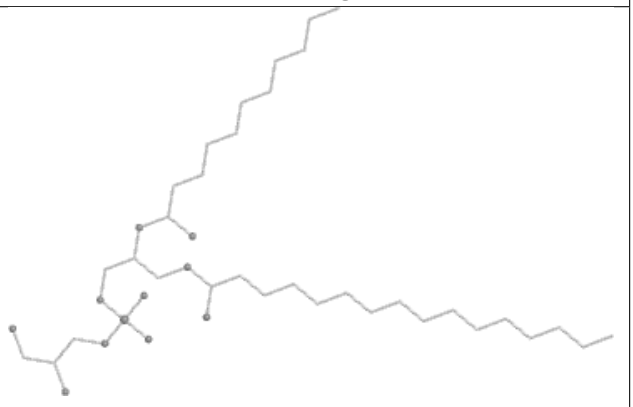
Bond lengths



Bond angles

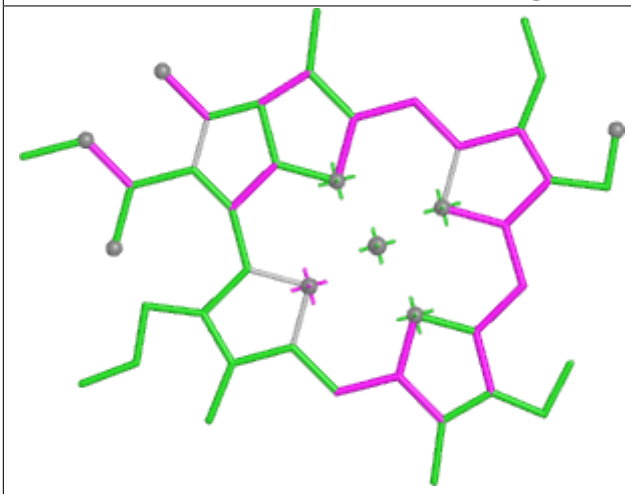


Torsions

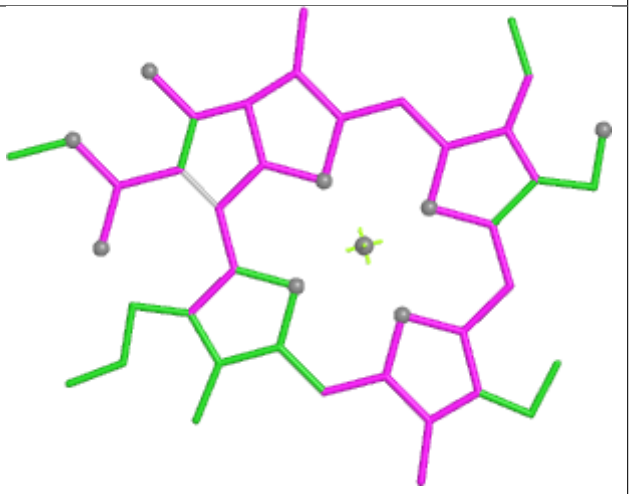


Rings

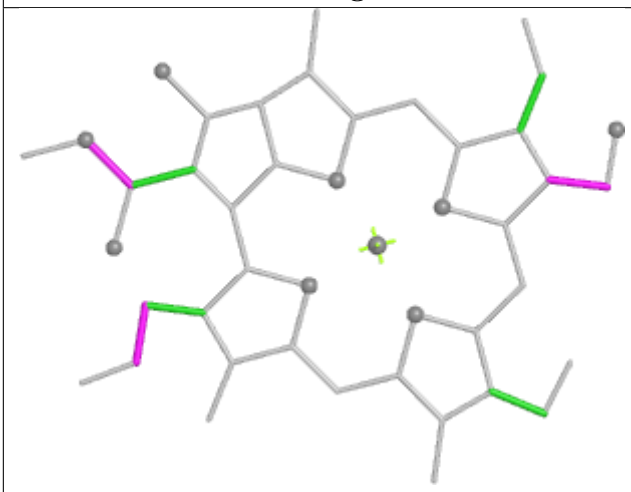
Ligand CHL 6 311



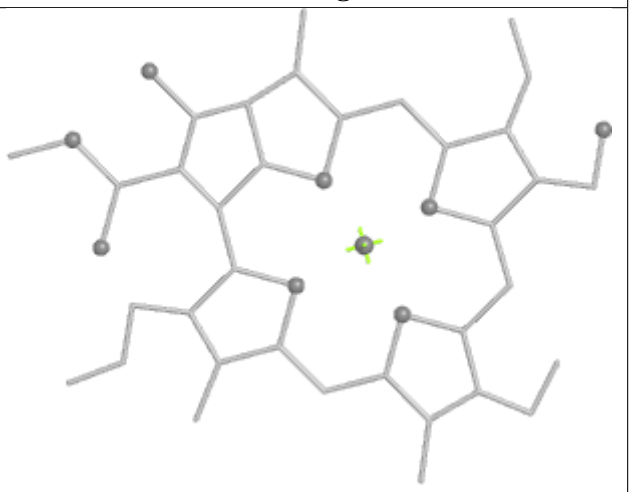
Bond lengths



Bond angles

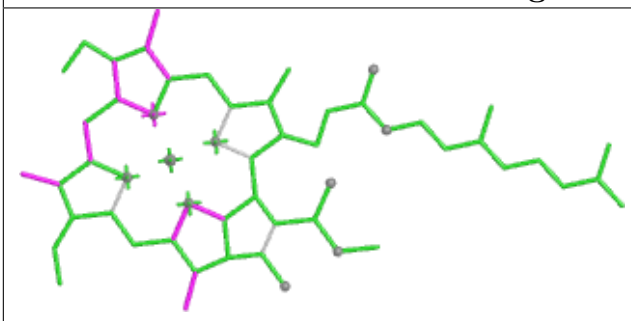


Torsions

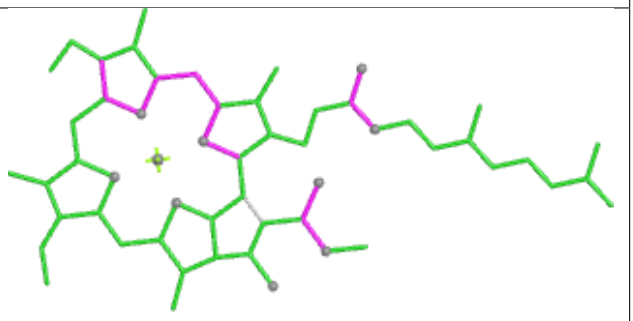


Rings

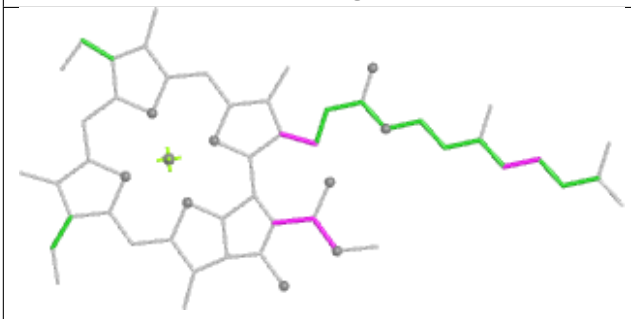
Ligand CLA 5 314



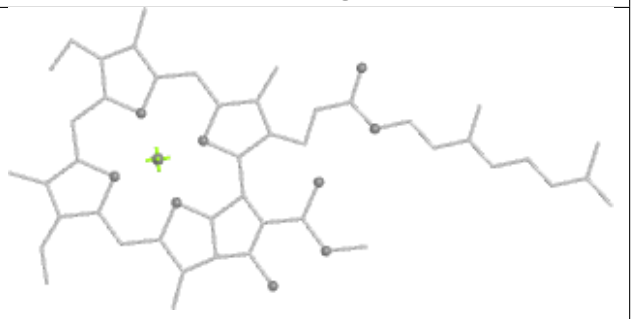
Bond lengths



Bond angles

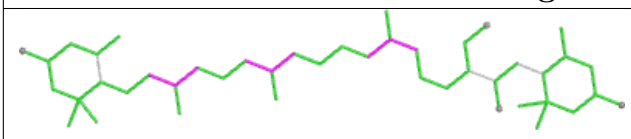


Torsions

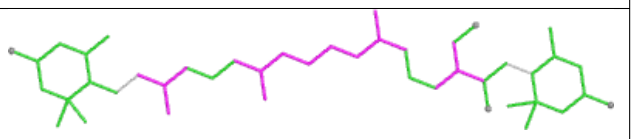


Rings

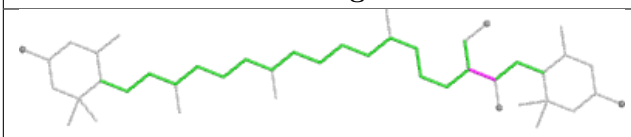
Ligand 0IE 4 302



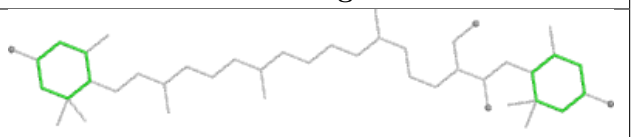
Bond lengths



Bond angles

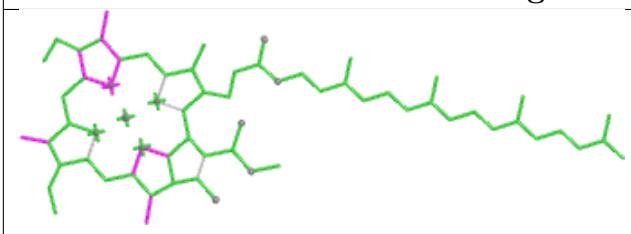


Torsions

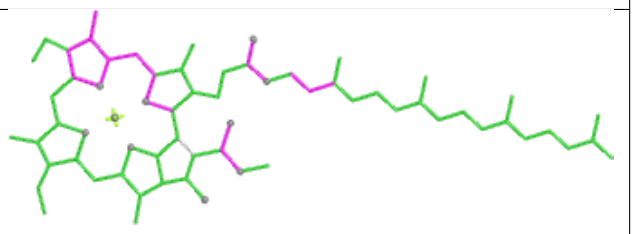


Rings

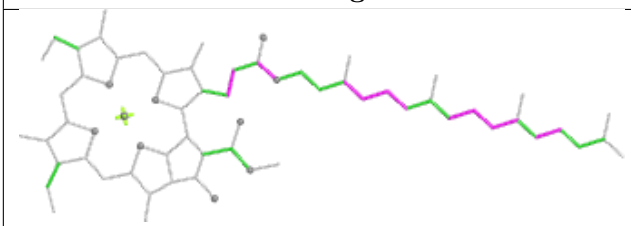
Ligand CLA b 612



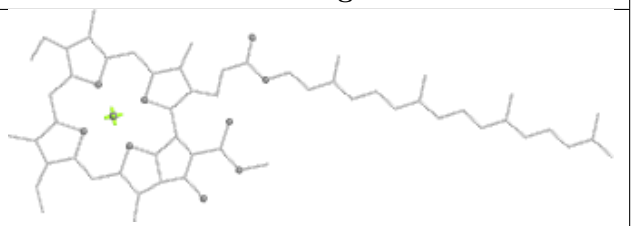
Bond lengths



Bond angles

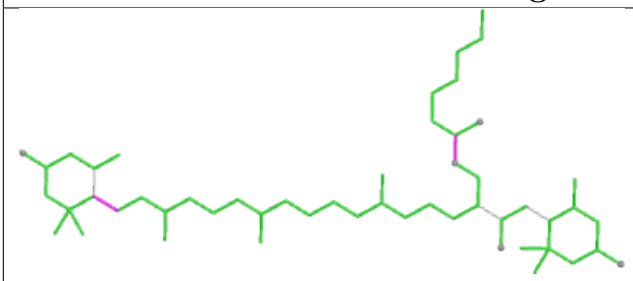


Torsions

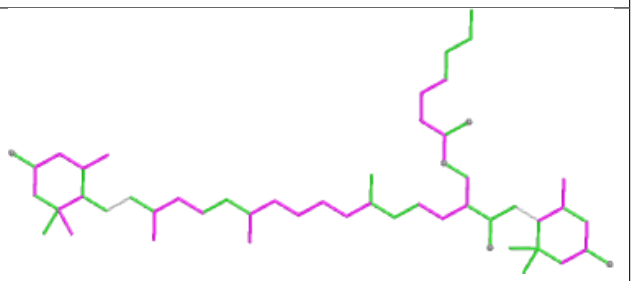


Rings

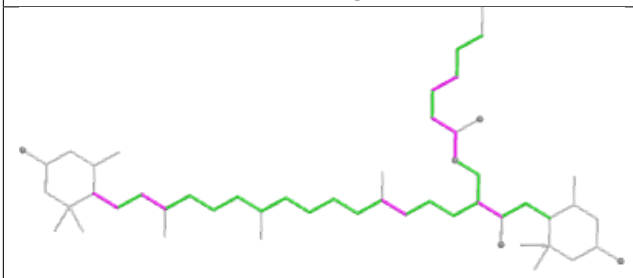
Ligand 0UR 2 301



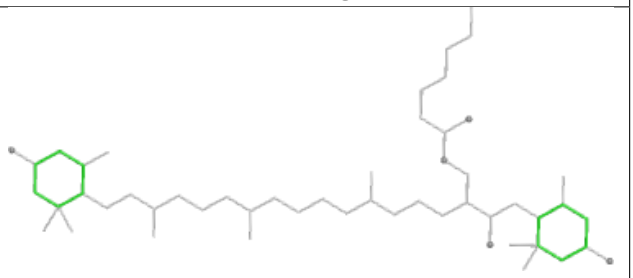
Bond lengths



Bond angles

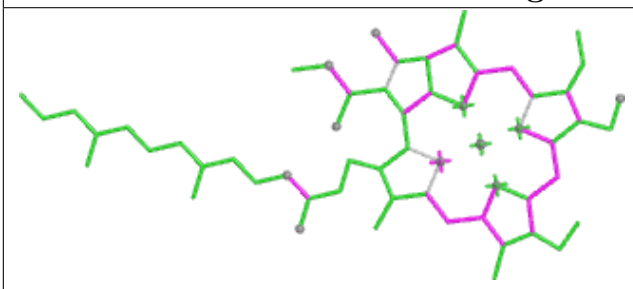


Torsions

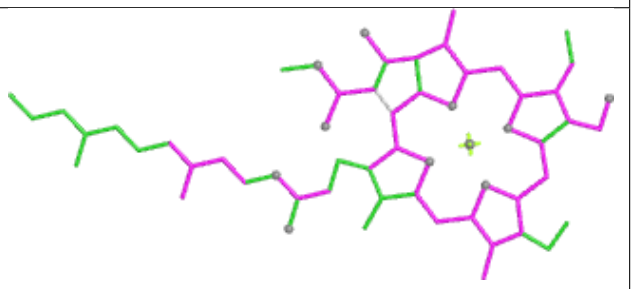


Rings

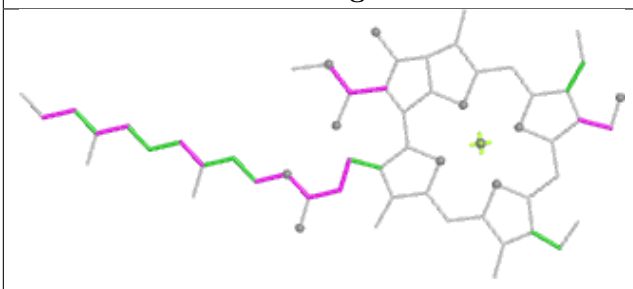
Ligand CHL S 602



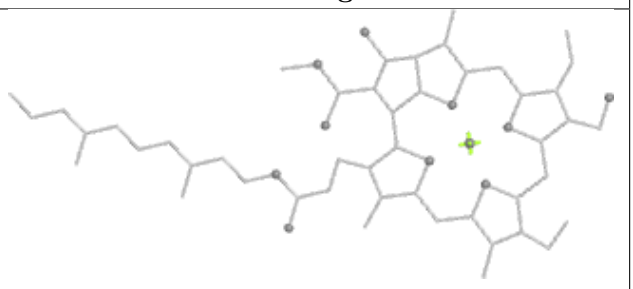
Bond lengths



Bond angles

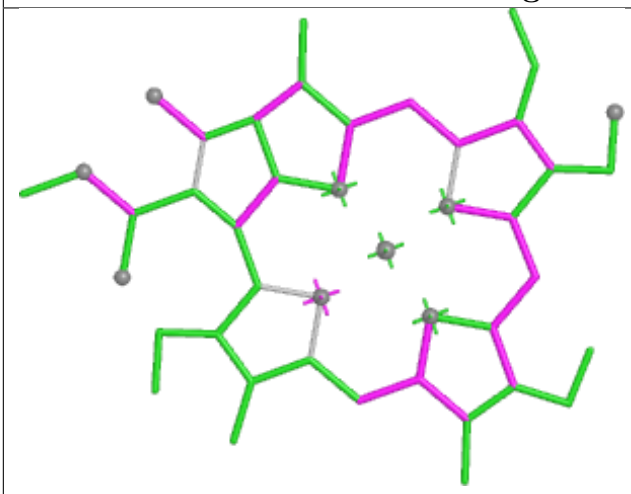


Torsions

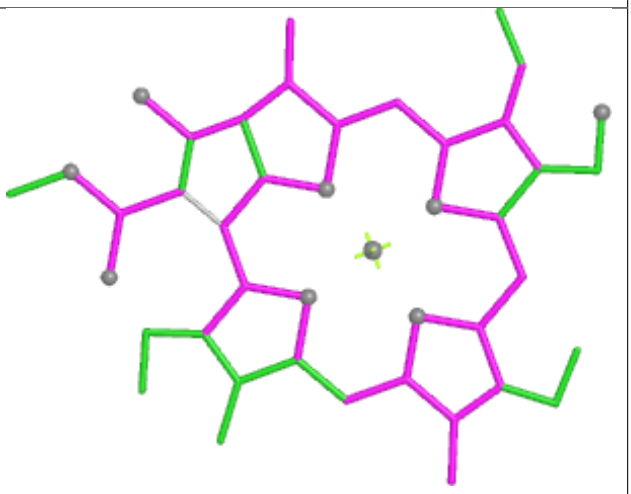


Rings

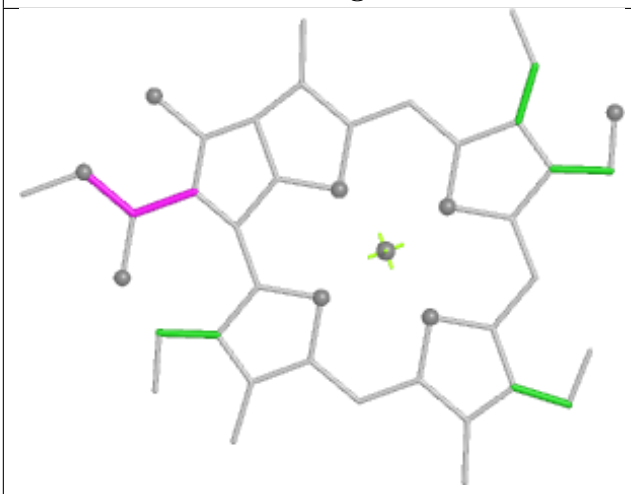
Ligand CHL N 308



Bond lengths



Bond angles

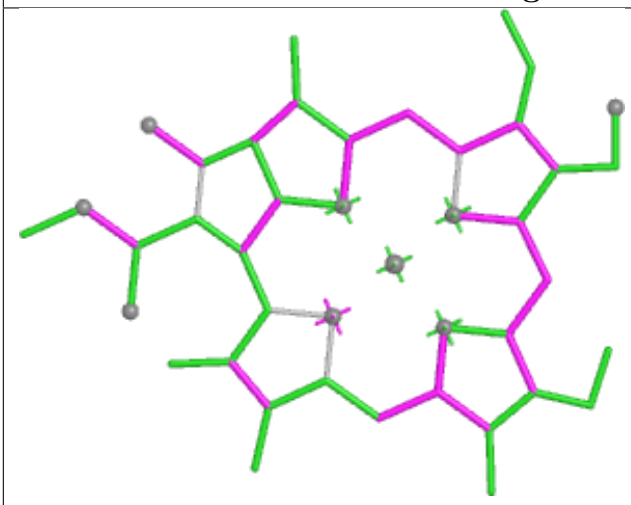


Torsions

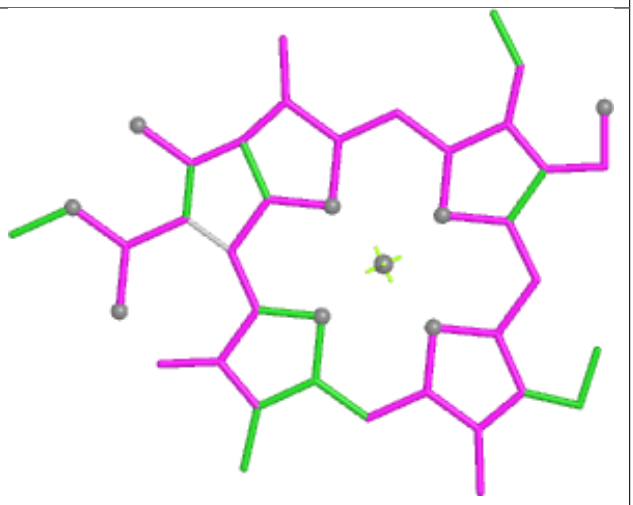


Rings

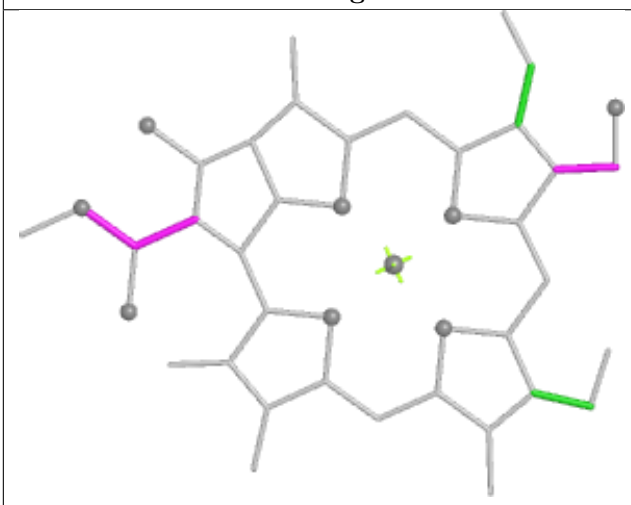
Ligand CHL G 318



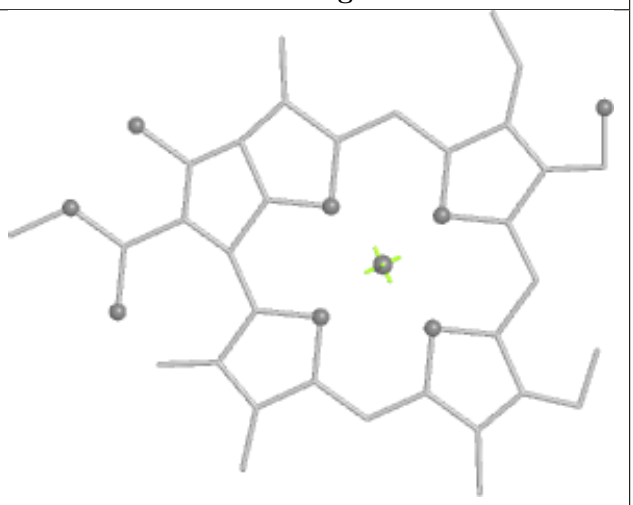
Bond lengths



Bond angles

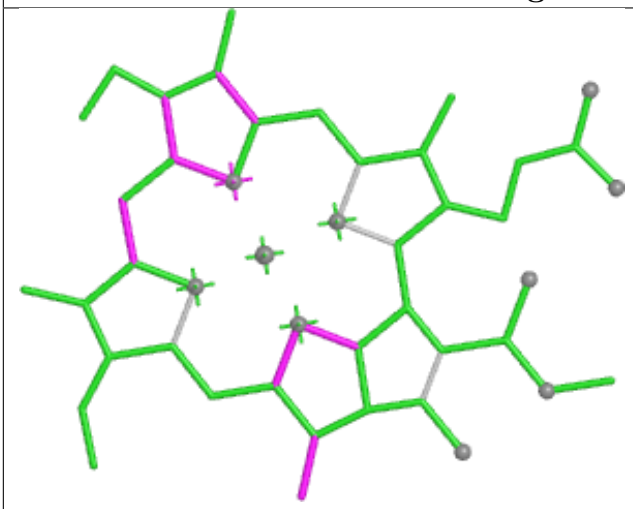


Torsions

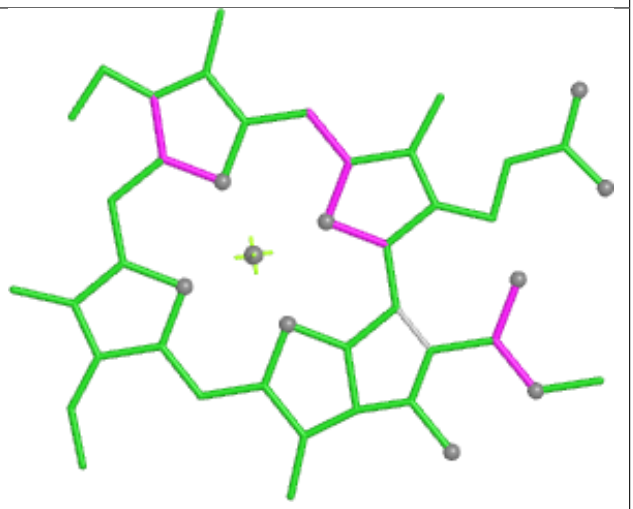


Rings

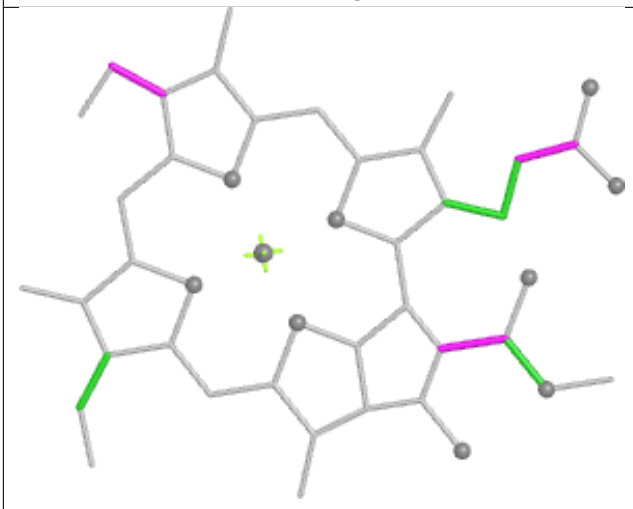
Ligand CLA u 316



Bond lengths



Bond angles

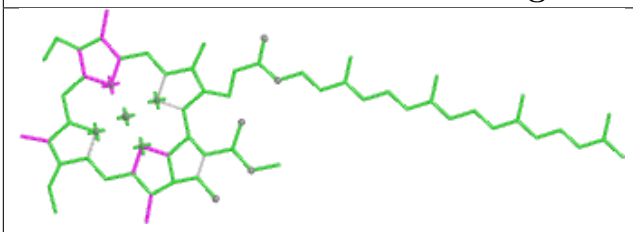


Torsions

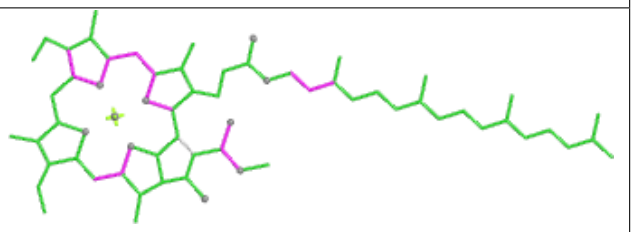


Rings

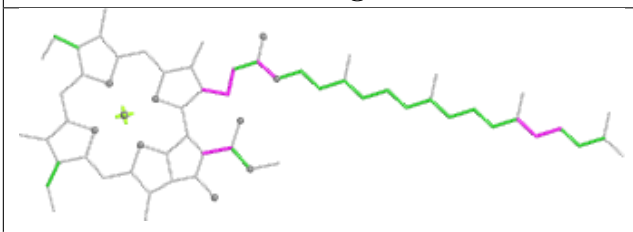
Ligand CLA a 604



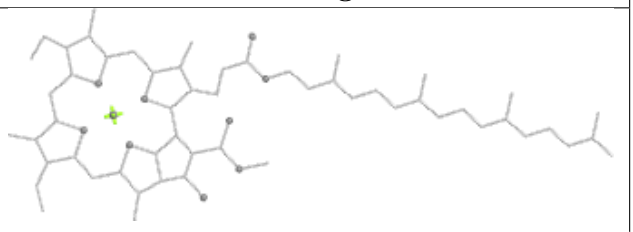
Bond lengths



Bond angles

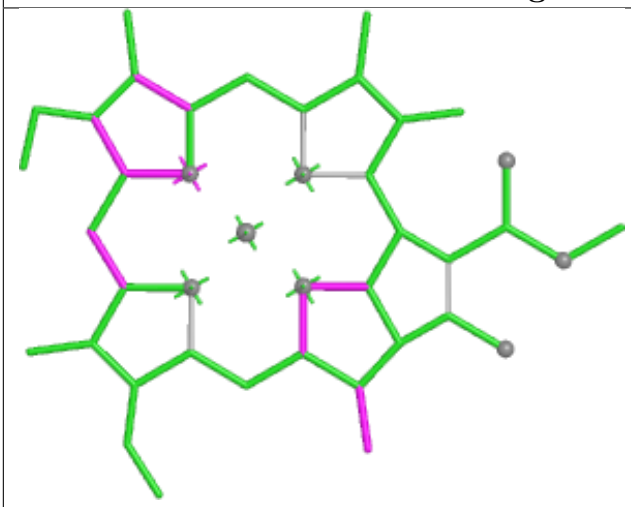


Torsions

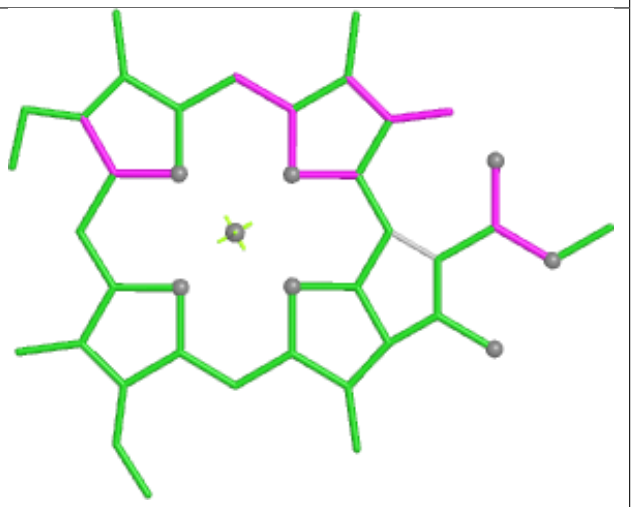


Rings

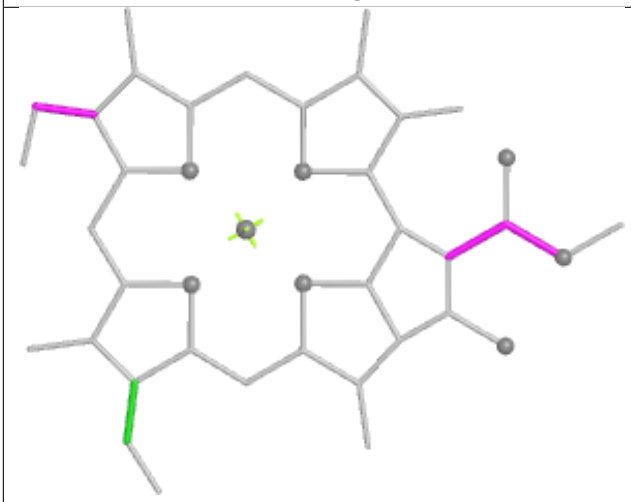
Ligand CLA 1 314



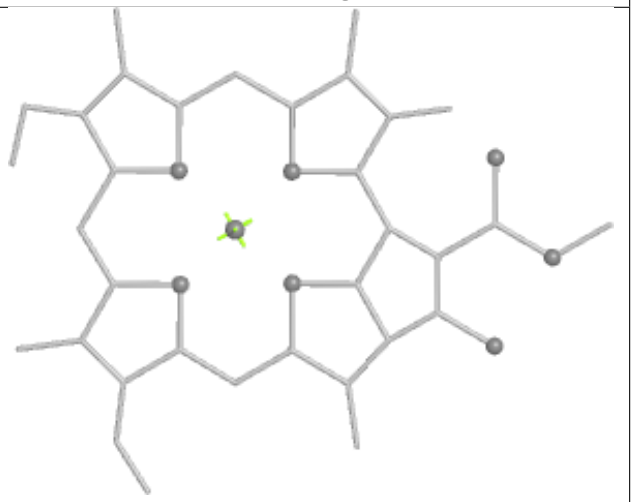
Bond lengths



Bond angles

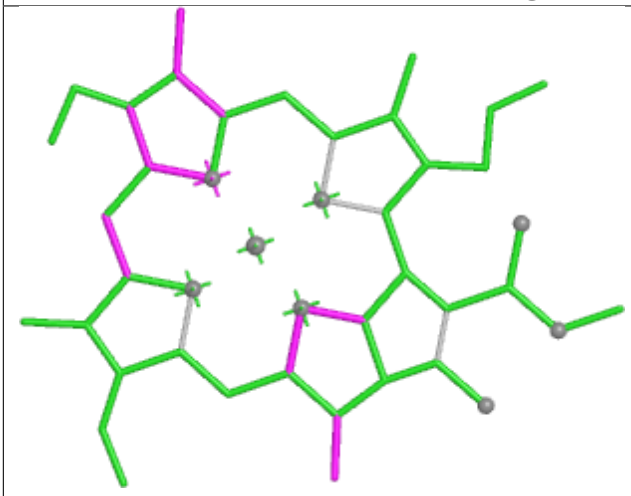


Torsions

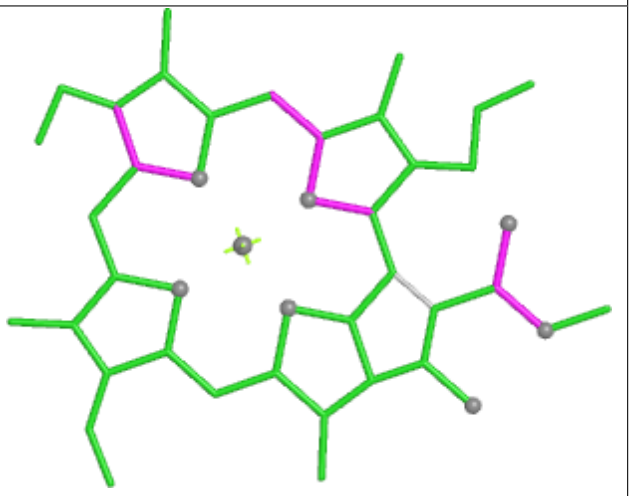


Rings

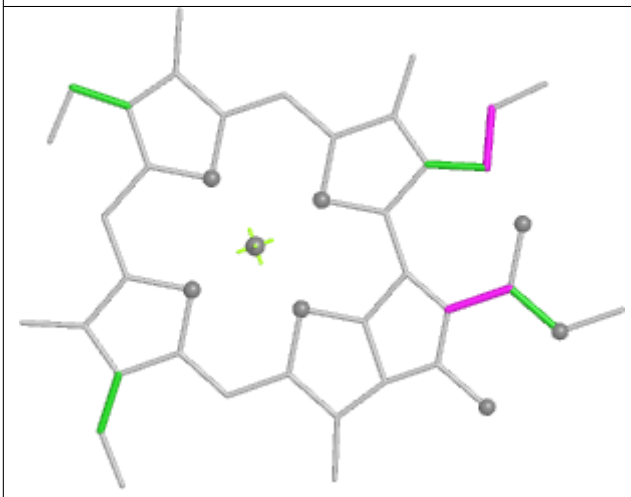
Ligand CLA N 316



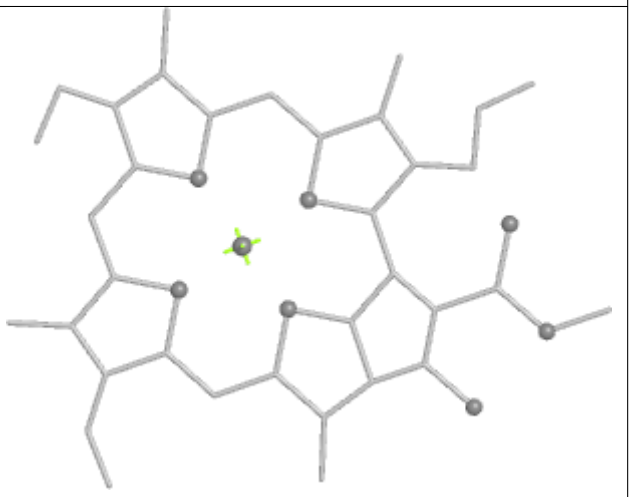
Bond lengths



Bond angles

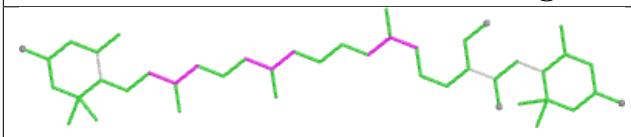


Torsions

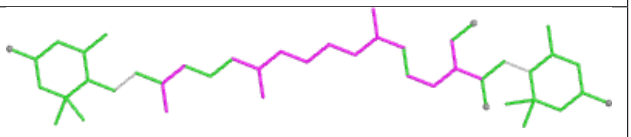


Rings

Ligand 0IE 9 302



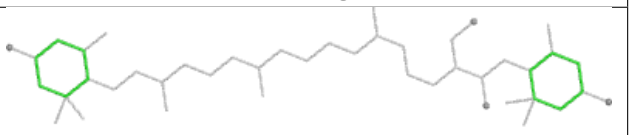
Bond lengths



Bond angles

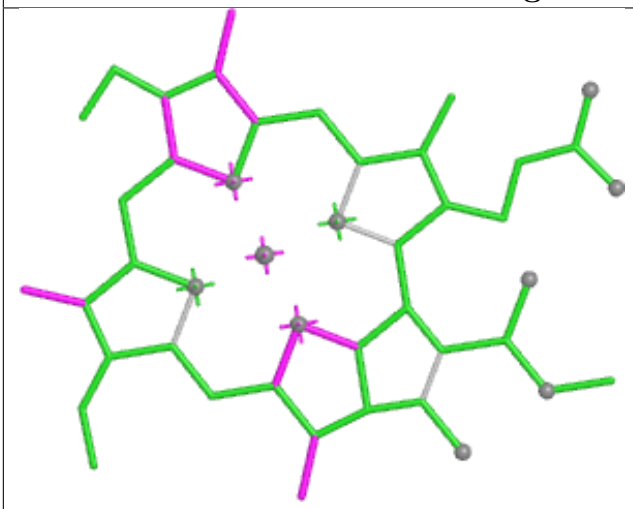


Torsions

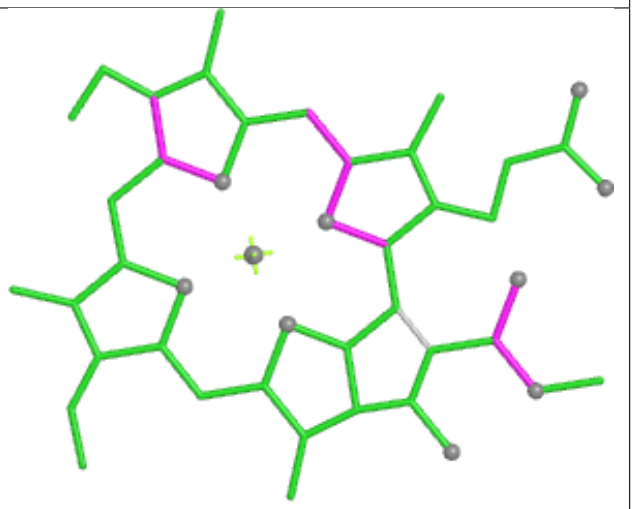


Rings

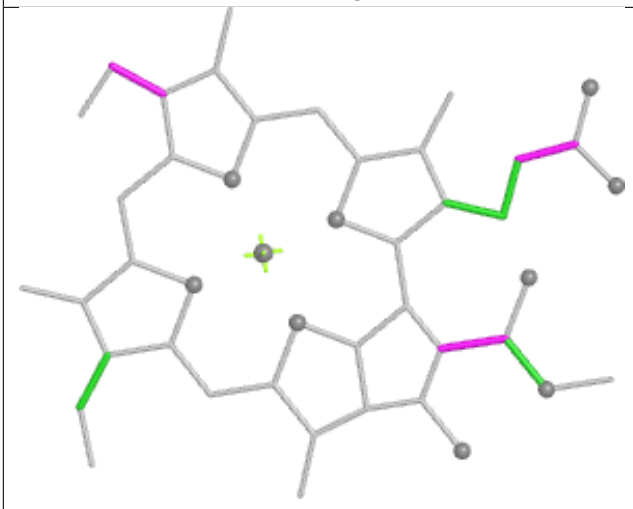
Ligand CLA Y 315



Bond lengths



Bond angles

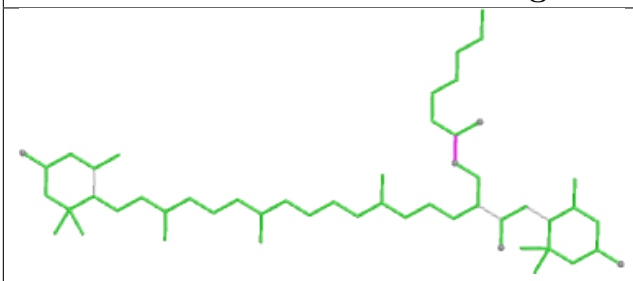


Torsions

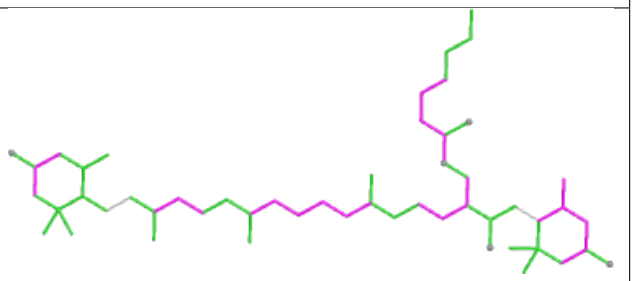


Rings

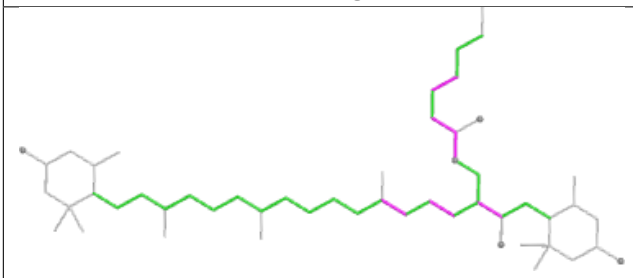
Ligand 0UR 3 301



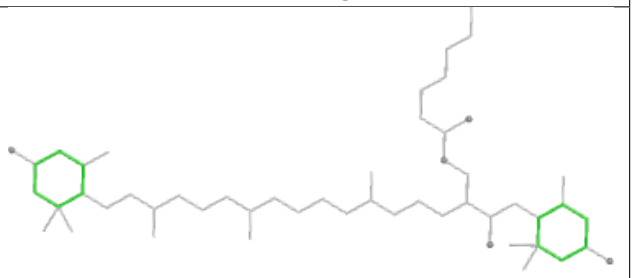
Bond lengths



Bond angles

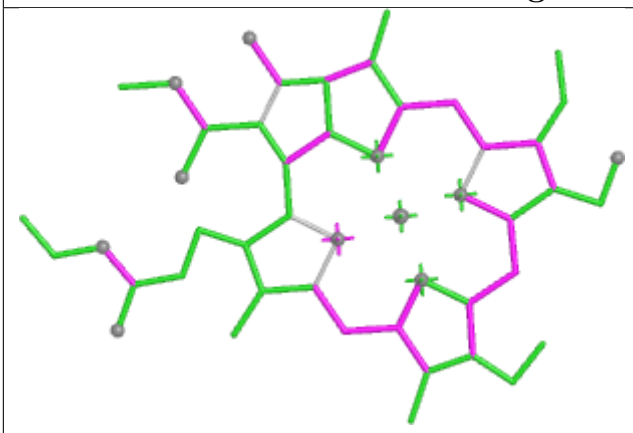


Torsions

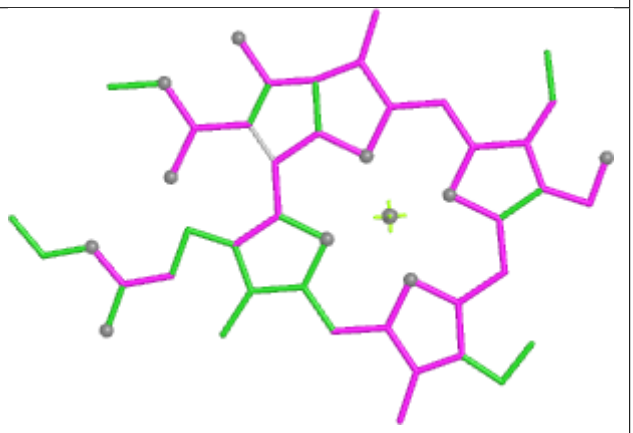


Rings

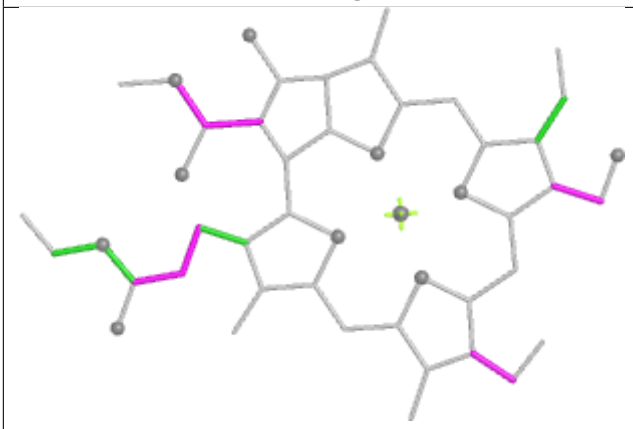
Ligand CHL 3 305



Bond lengths



Bond angles

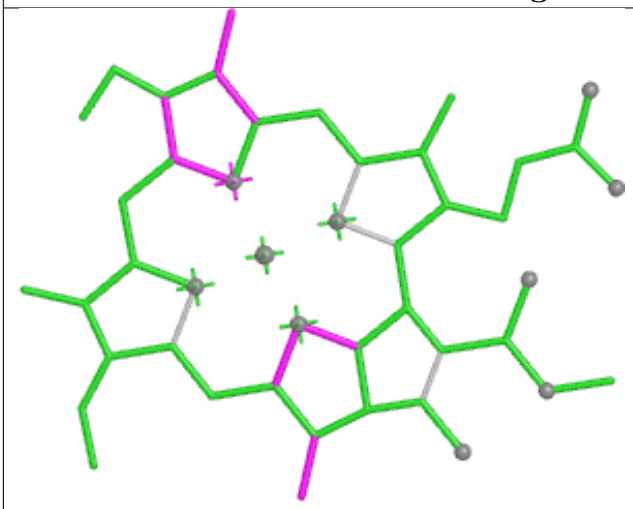


Torsions

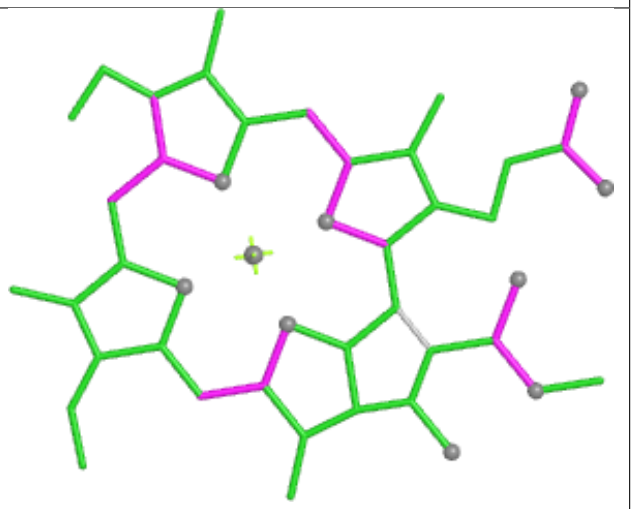


Rings

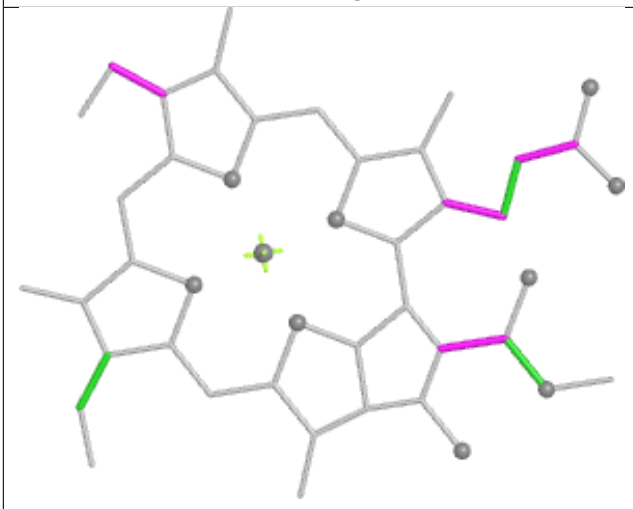
Ligand CLA r 313



Bond lengths



Bond angles

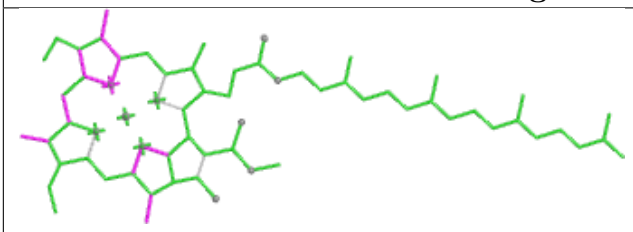


Torsions

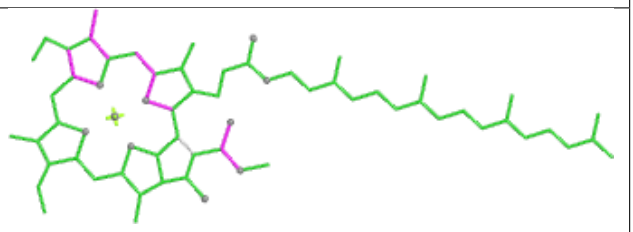


Rings

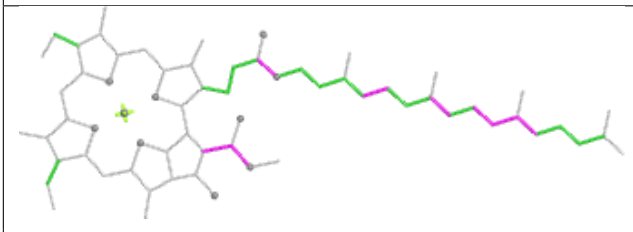
Ligand CLA c 611



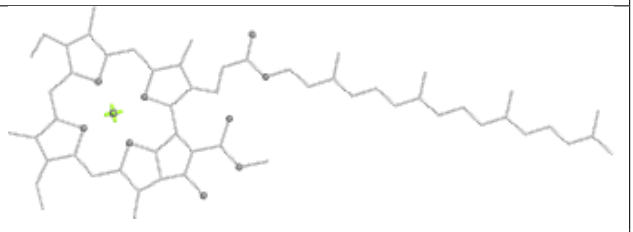
Bond lengths



Bond angles

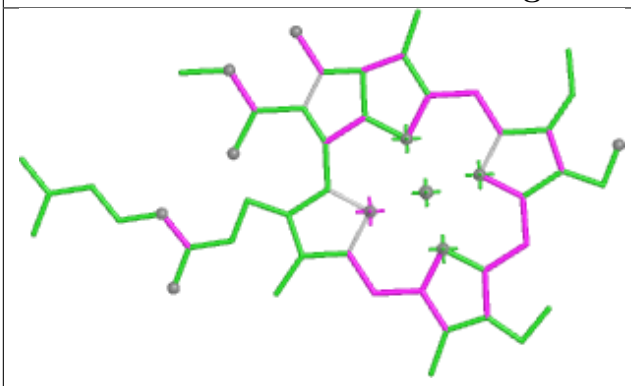


Torsions

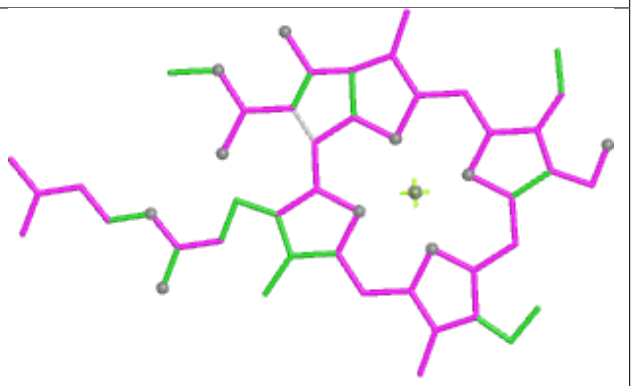


Rings

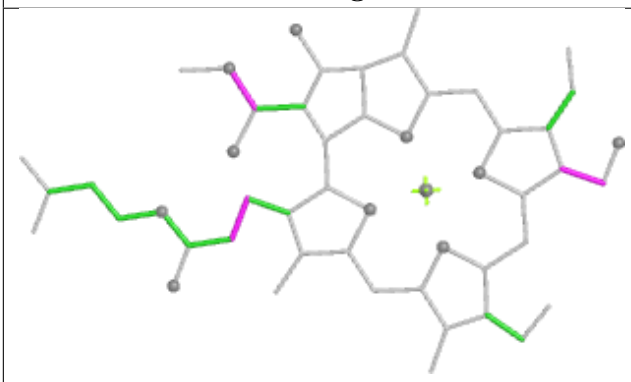
Ligand CHL Y 311



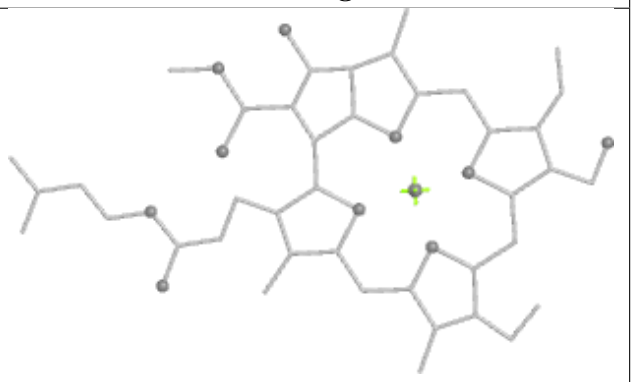
Bond lengths



Bond angles

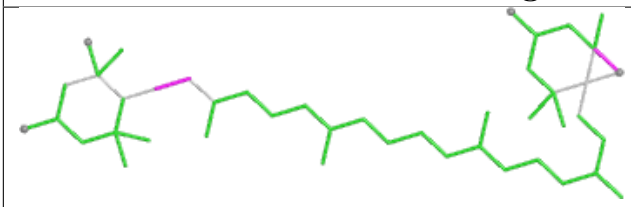


Torsions



Rings

Ligand NEX R 616



Bond lengths



Bond angles

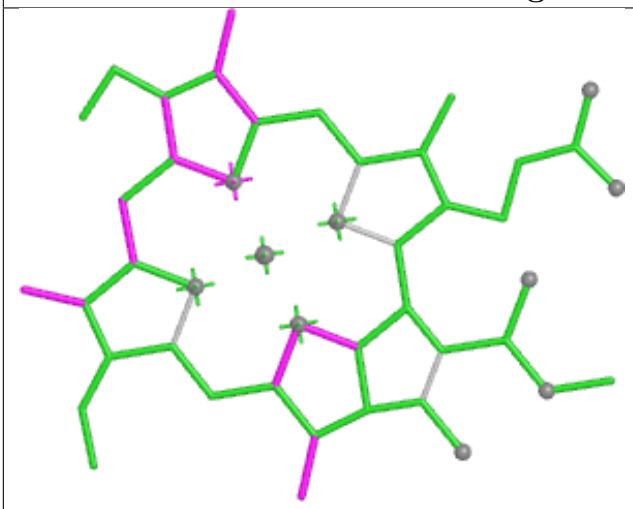


Torsions

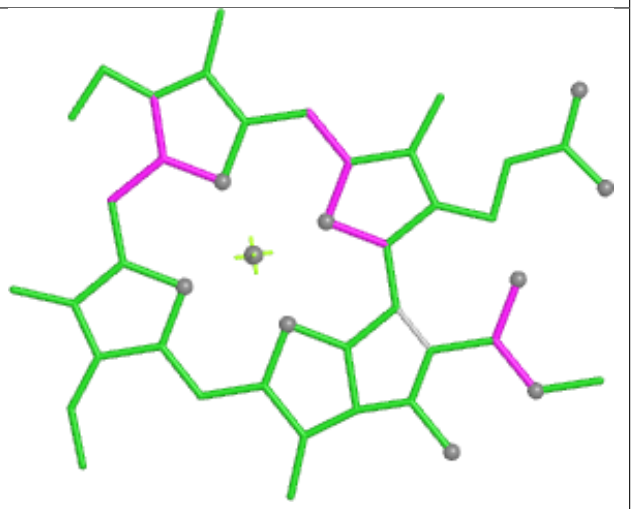


Rings

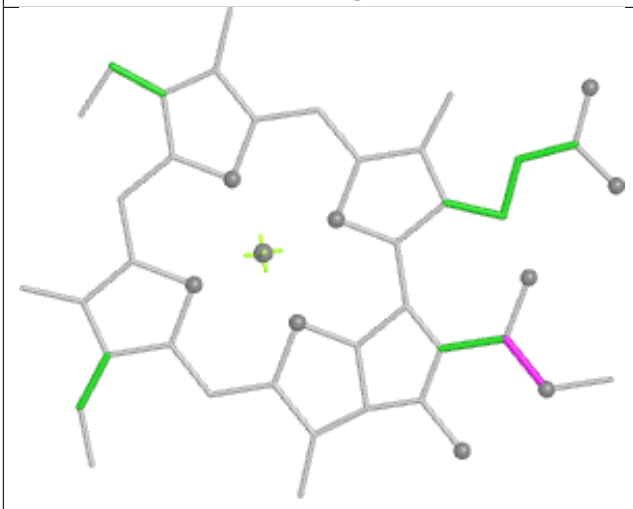
Ligand CLA S 610



Bond lengths



Bond angles

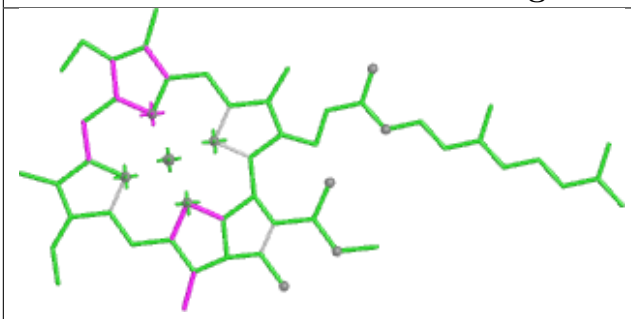


Torsions

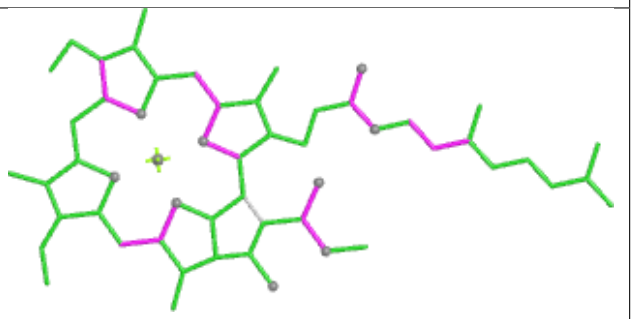


Rings

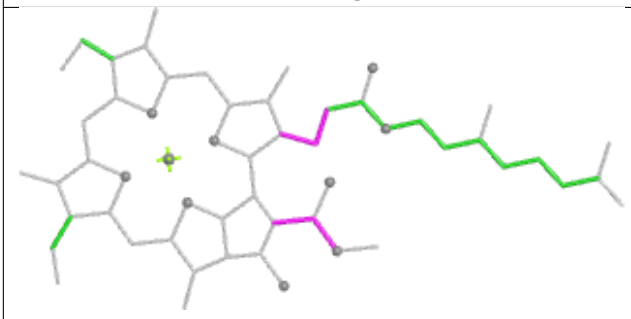
Ligand CLA 1 313



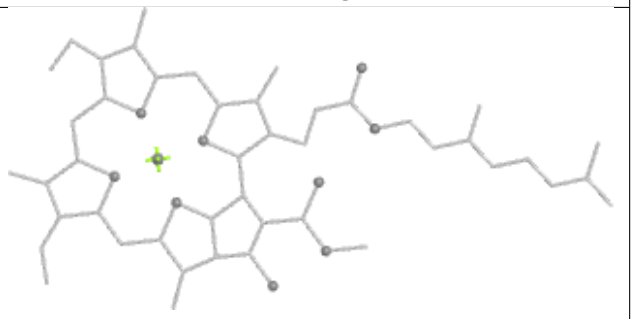
Bond lengths



Bond angles

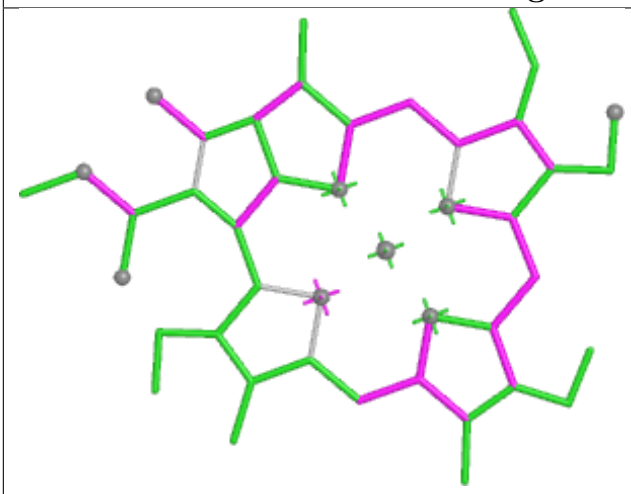


Torsions

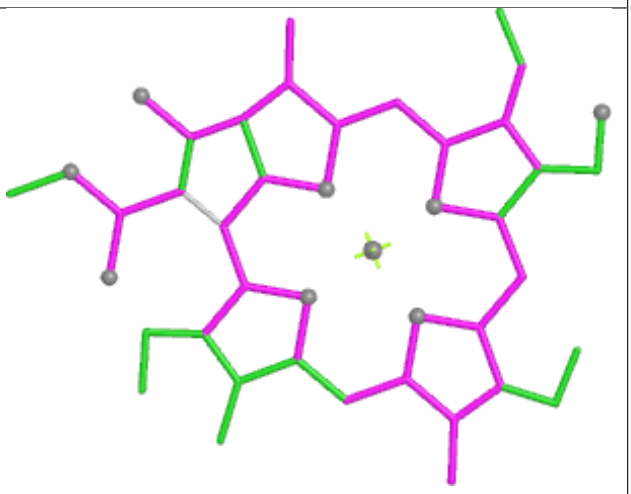


Rings

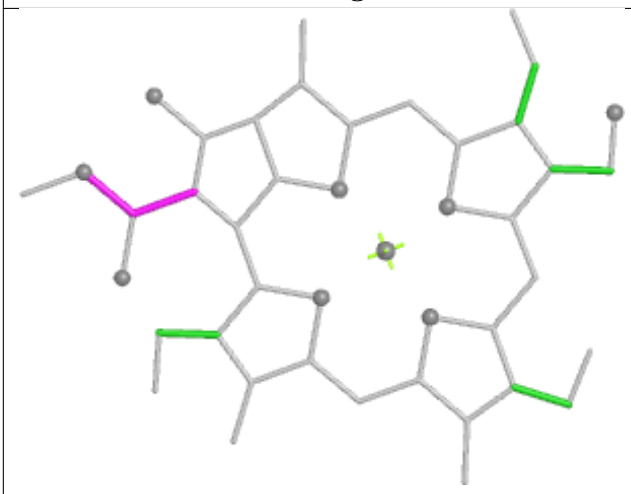
Ligand CHL 9 312



Bond lengths



Bond angles

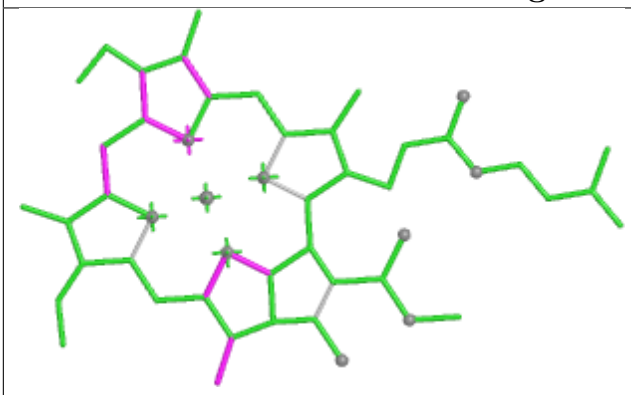


Torsions

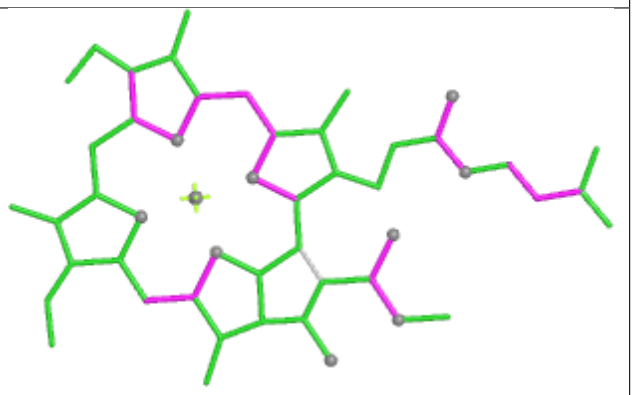


Rings

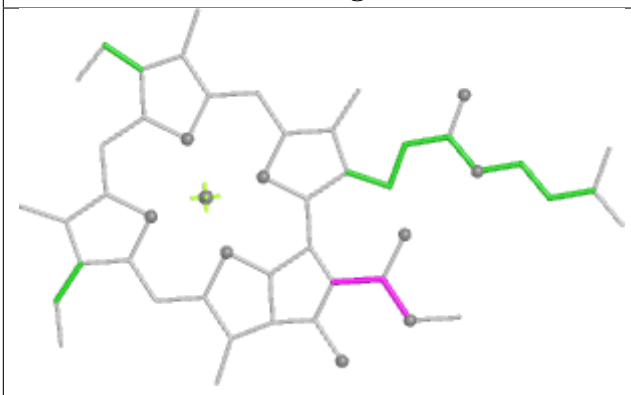
Ligand CLA 5 308



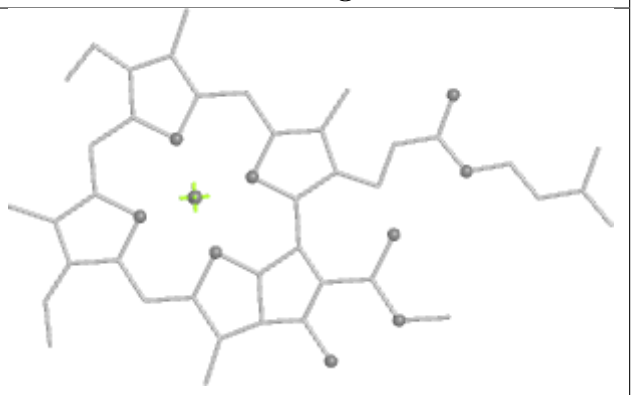
Bond lengths



Bond angles

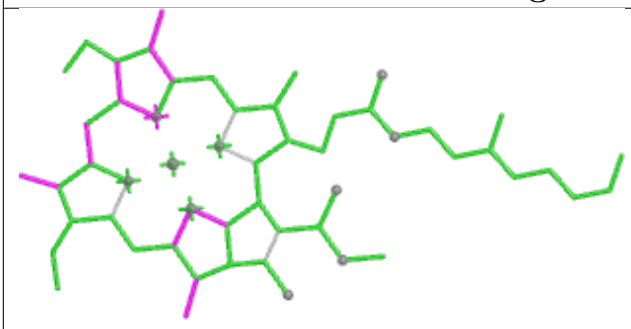


Torsions

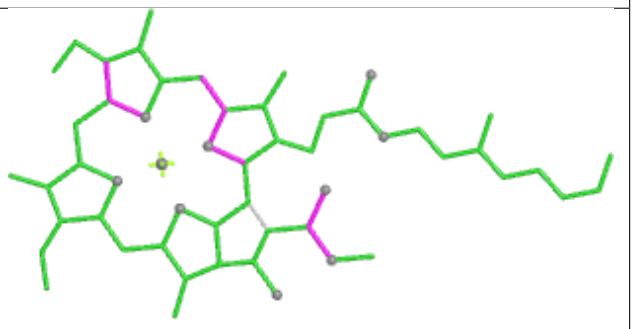


Rings

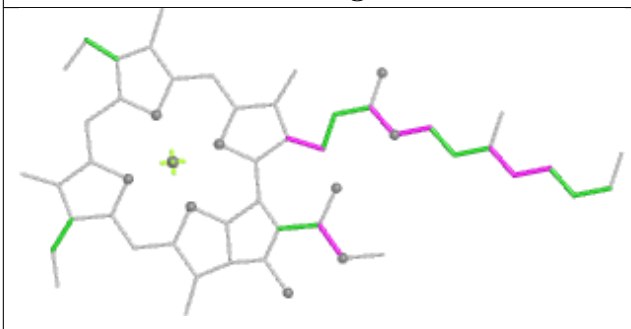
Ligand CLA c 612



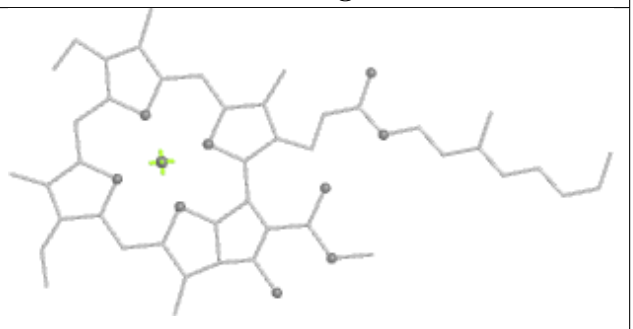
Bond lengths



Bond angles

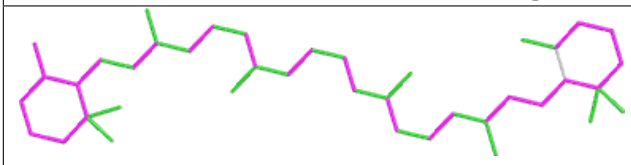


Torsions

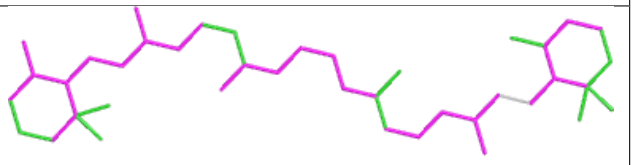


Rings

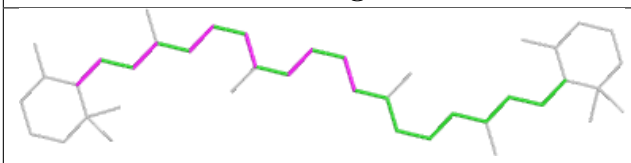
Ligand 8CT A 608



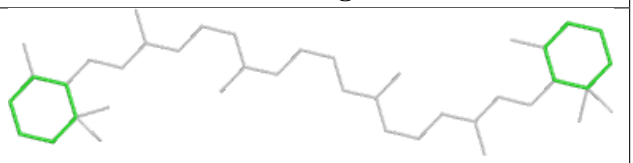
Bond lengths



Bond angles

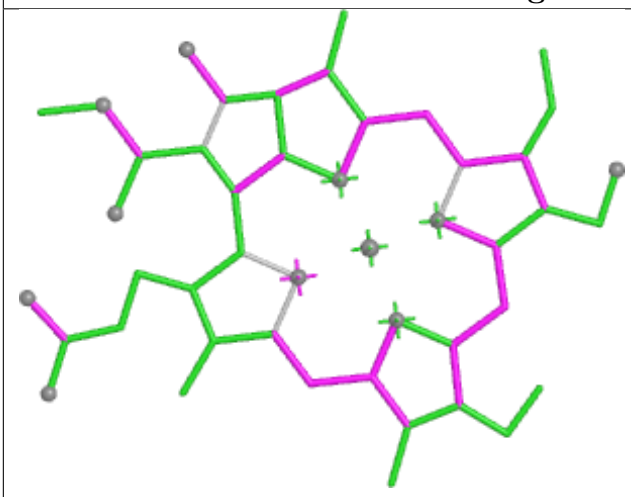


Torsions

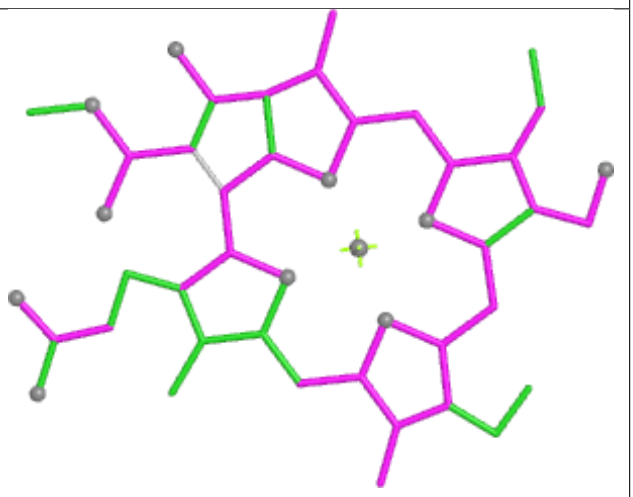


Rings

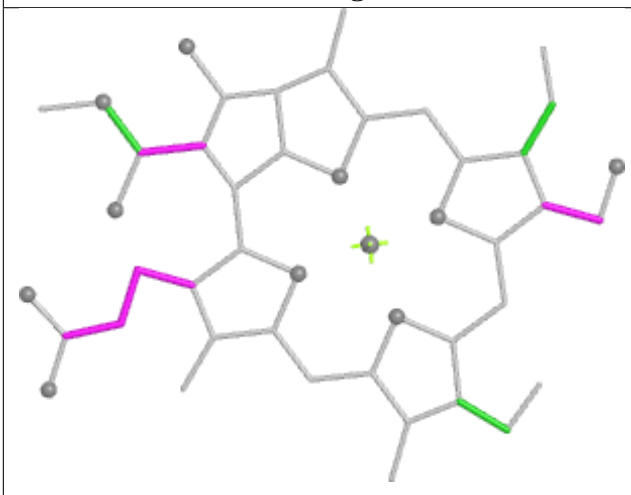
Ligand CHL 1 305



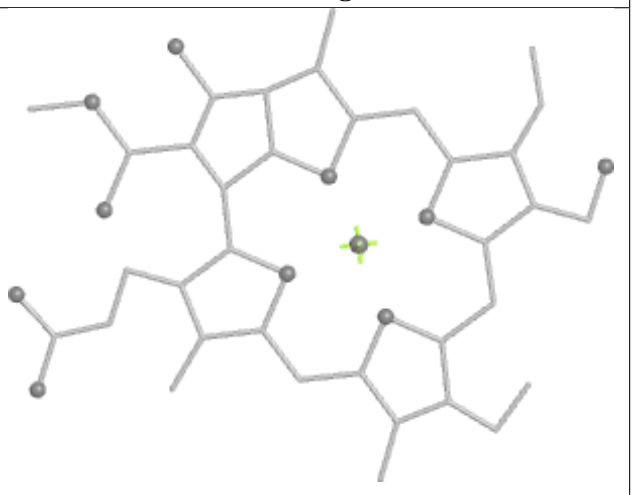
Bond lengths



Bond angles

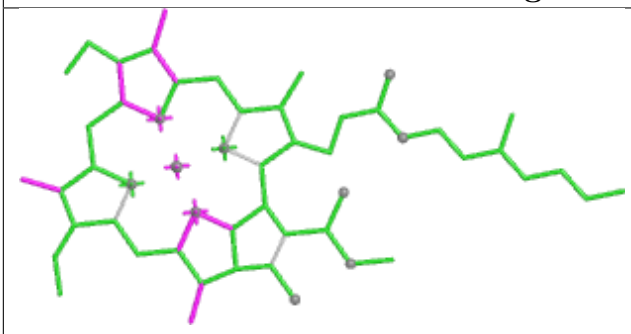


Torsions

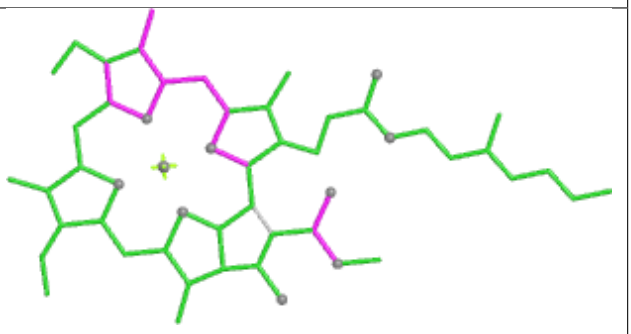


Rings

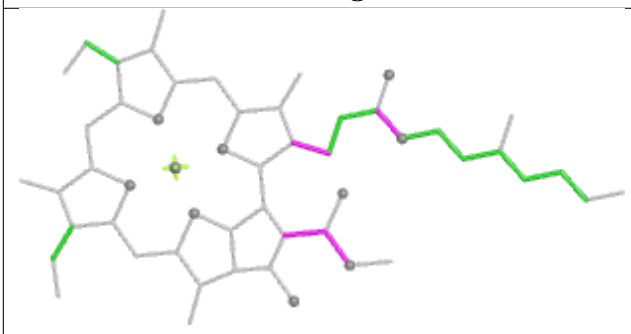
Ligand CLA C 606



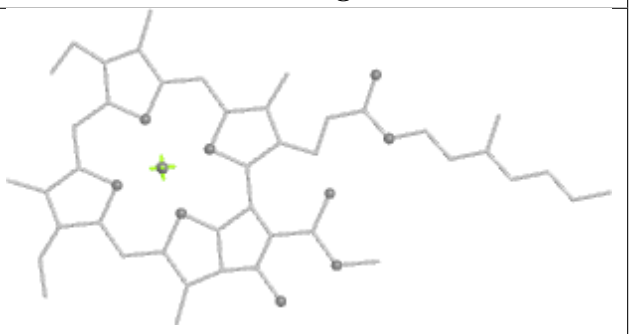
Bond lengths



Bond angles

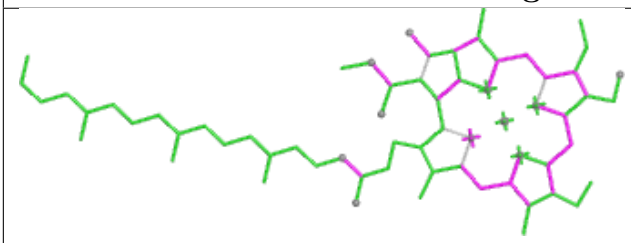


Torsions

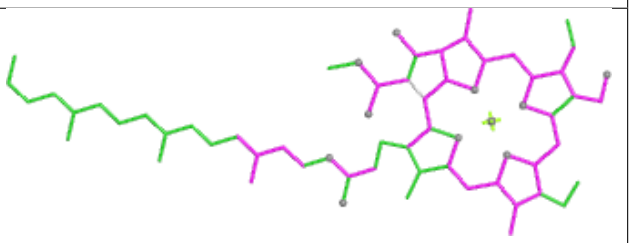


Rings

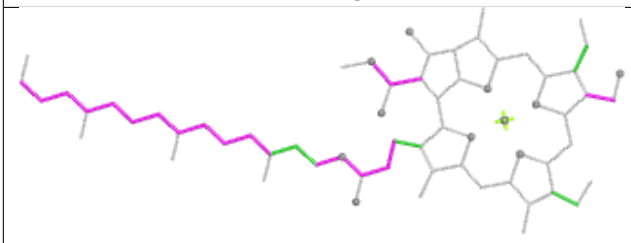
Ligand CHL G 306



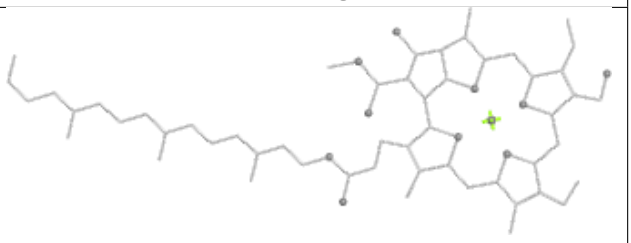
Bond lengths



Bond angles

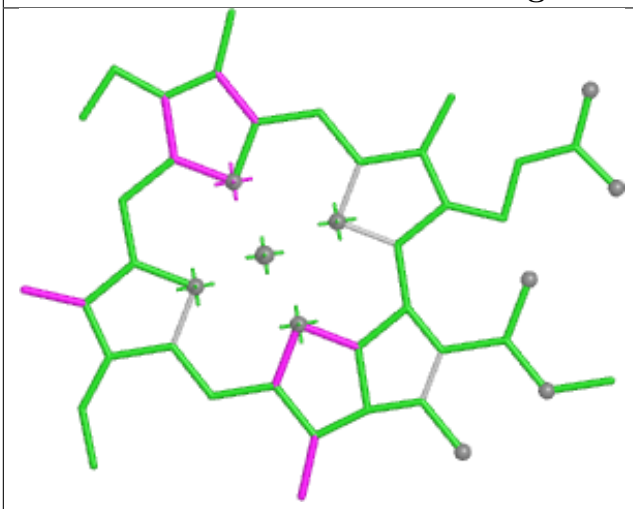


Torsions

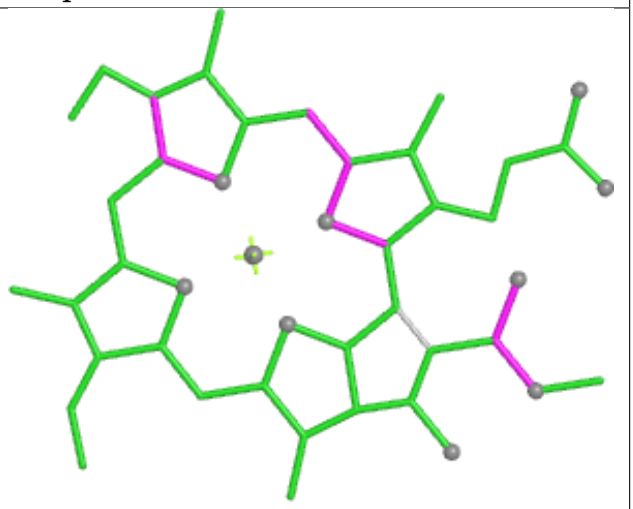


Rings

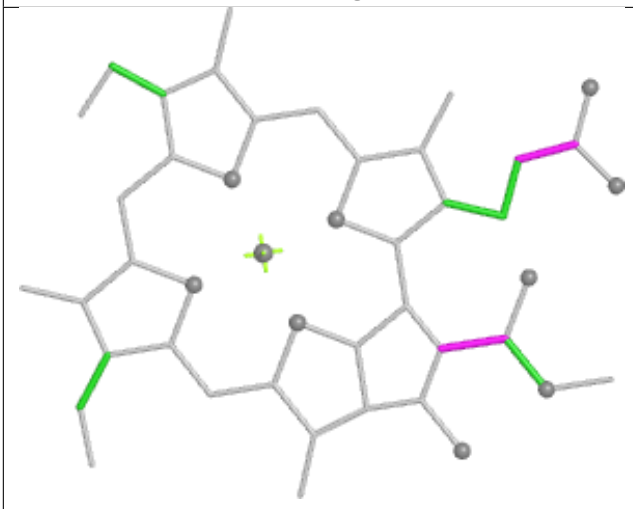
Ligand CLA q 314



Bond lengths



Bond angles

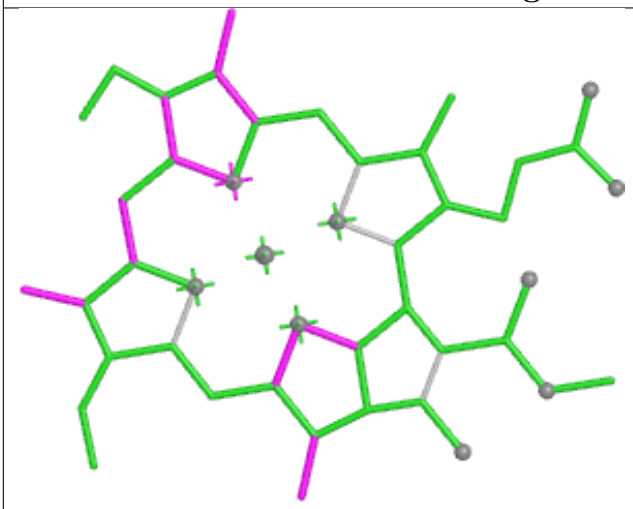


Torsions

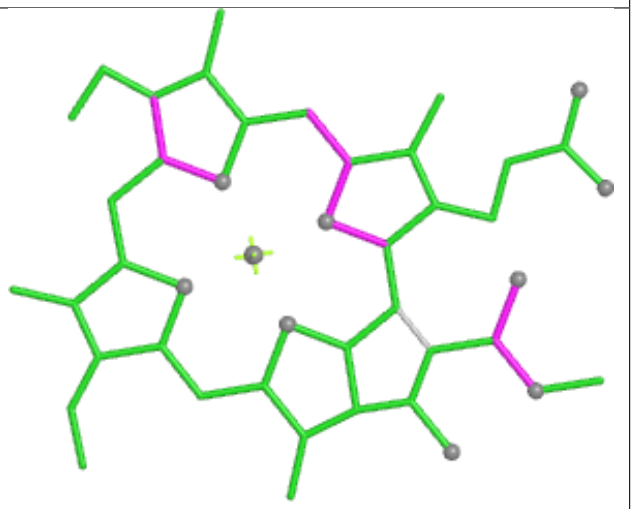


Rings

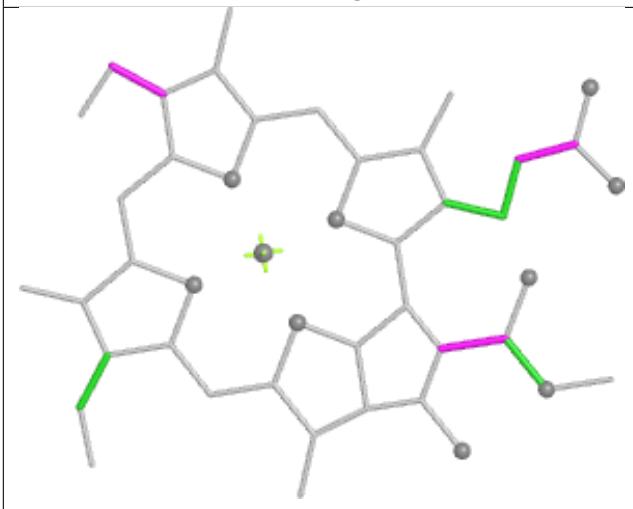
Ligand CLA G 316



Bond lengths



Bond angles

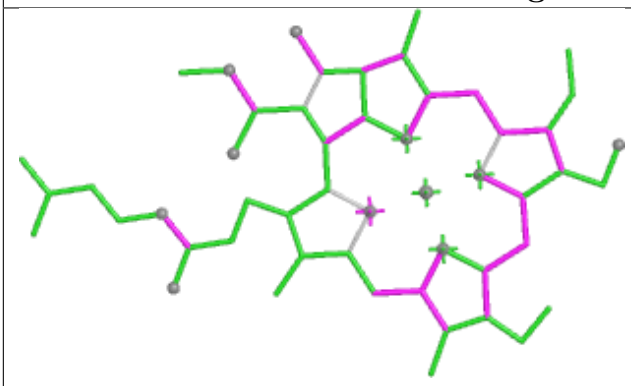


Torsions

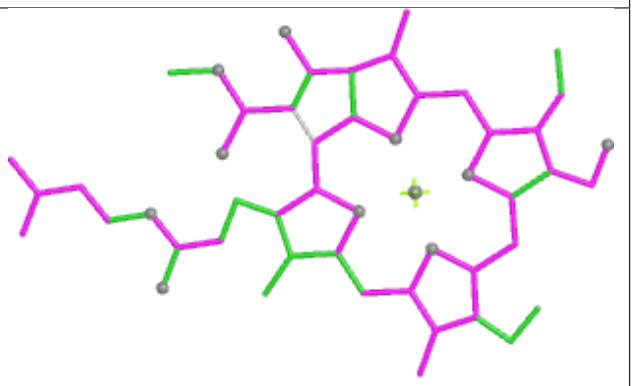


Rings

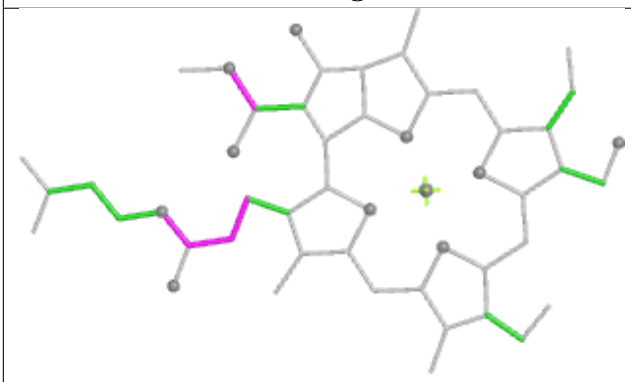
Ligand CHL 6 309



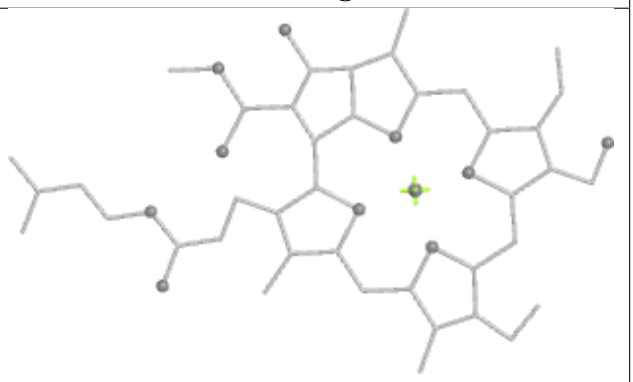
Bond lengths



Bond angles

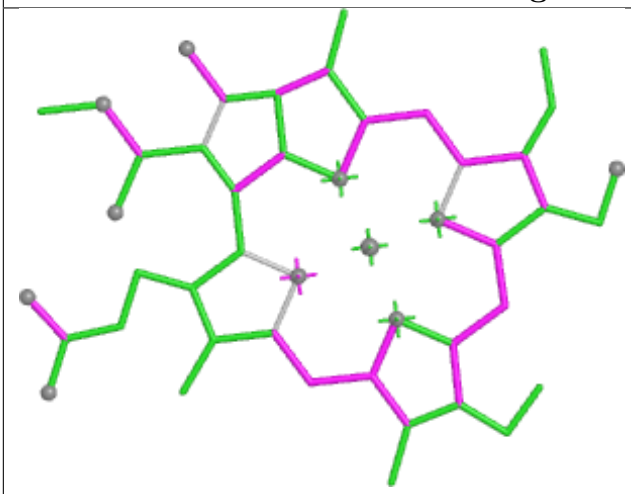


Torsions

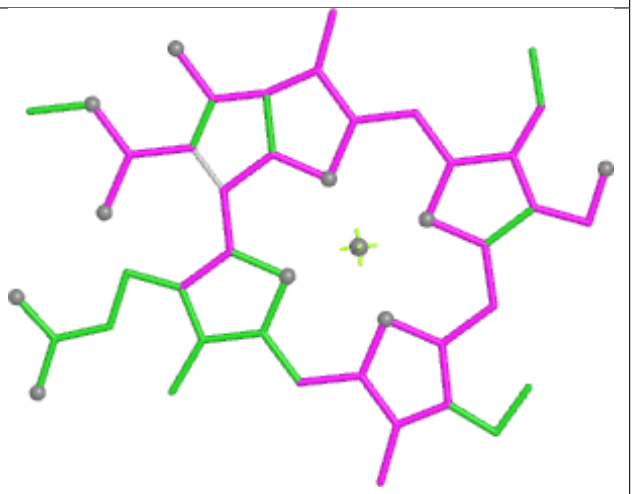


Rings

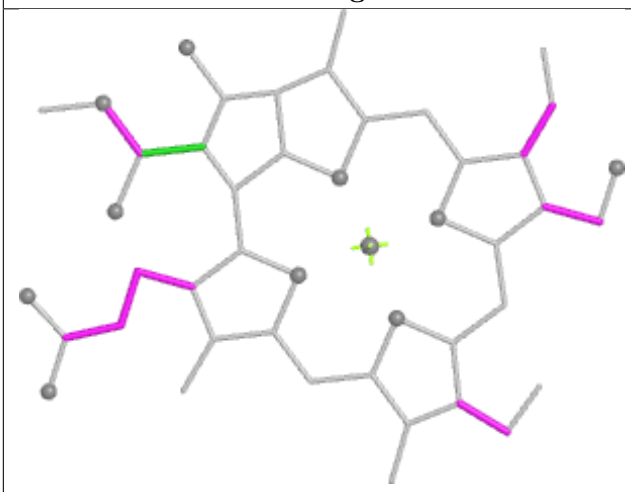
Ligand CHL s 402



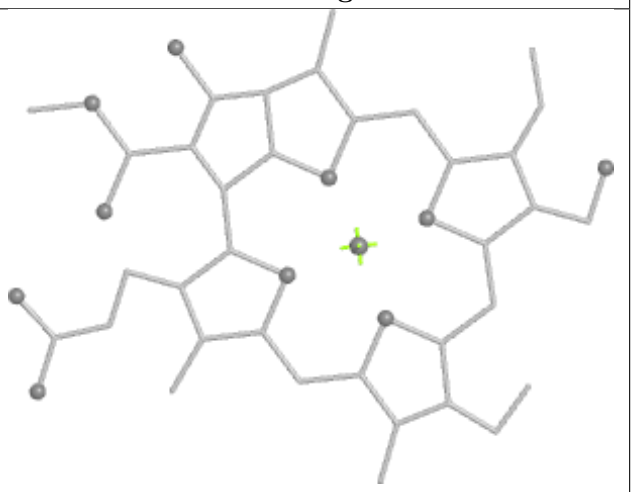
Bond lengths



Bond angles

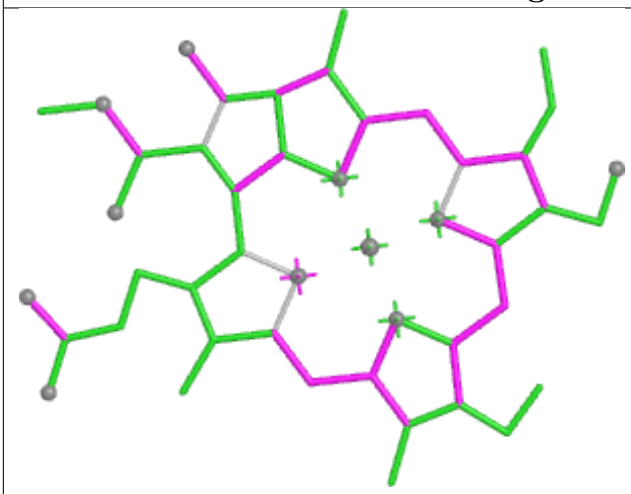


Torsions

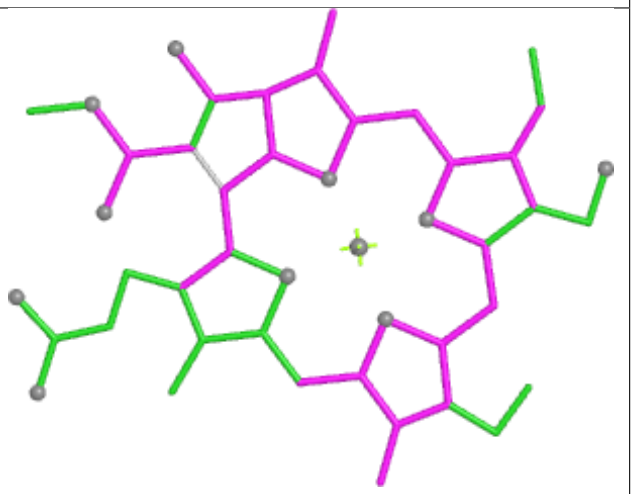


Rings

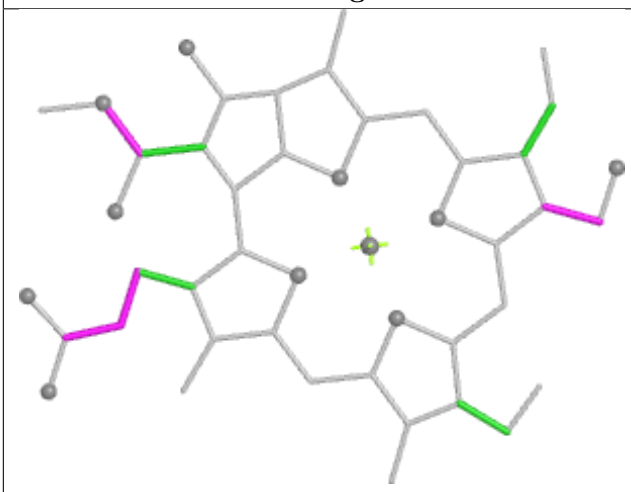
Ligand CHL 2 312



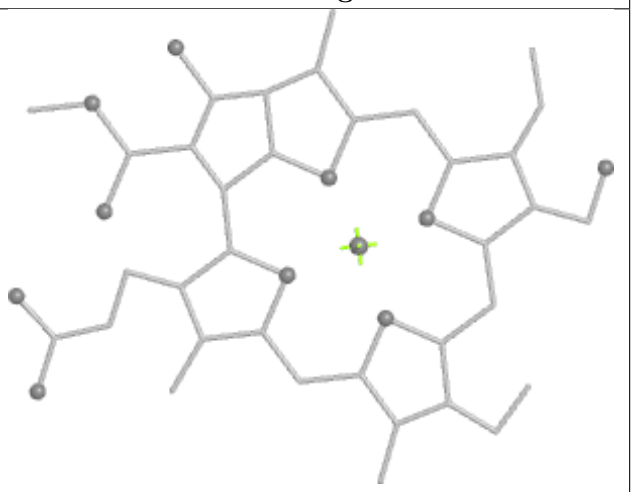
Bond lengths



Bond angles

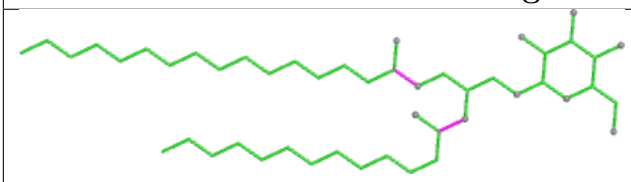


Torsions

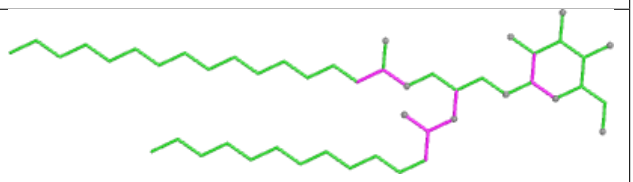


Rings

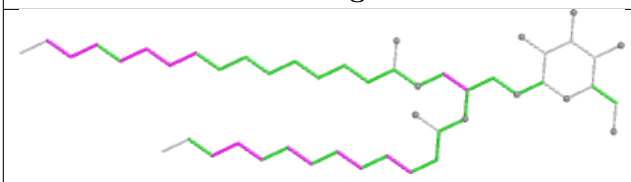
Ligand LMG d 401



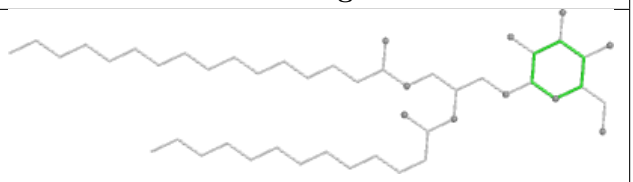
Bond lengths



Bond angles

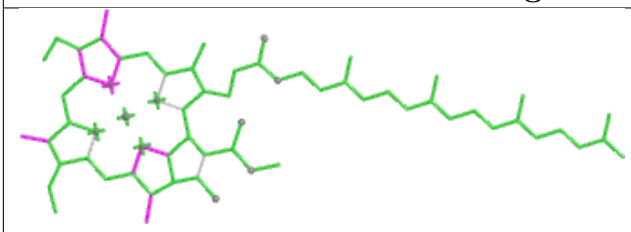


Torsions

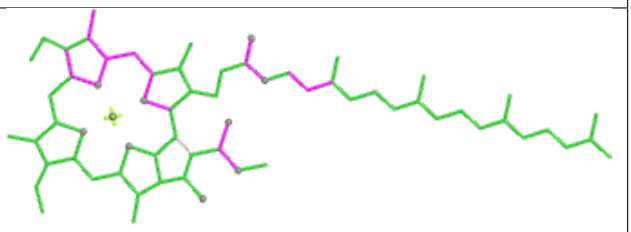


Rings

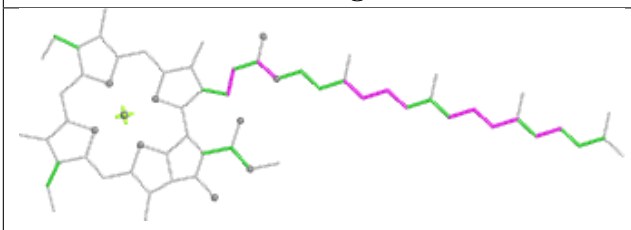
Ligand CLA B 612



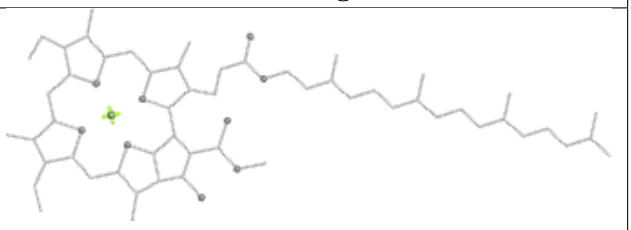
Bond lengths



Bond angles

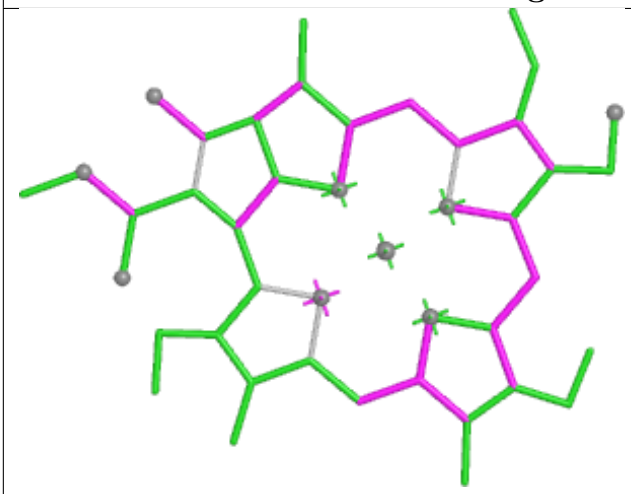


Torsions

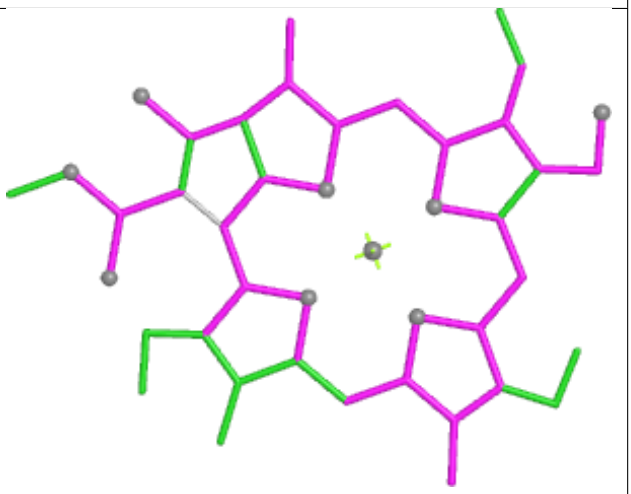


Rings

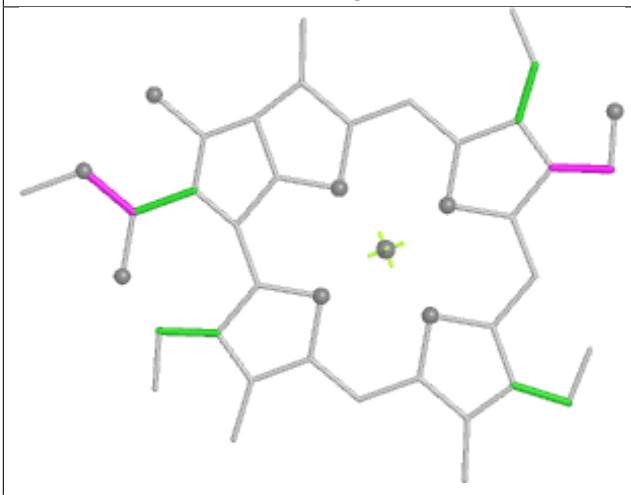
Ligand CHL 4 309



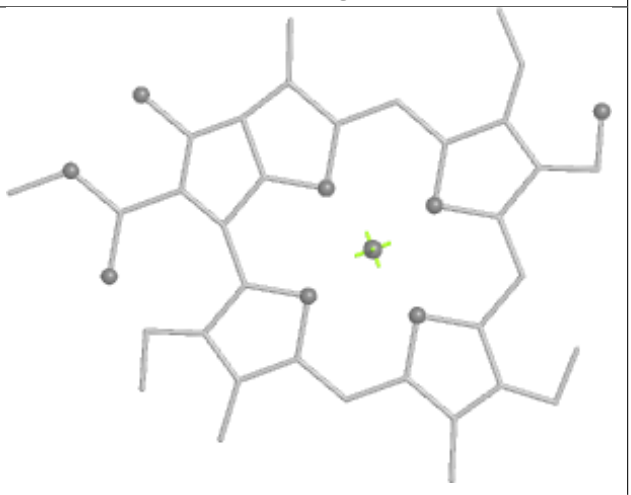
Bond lengths



Bond angles

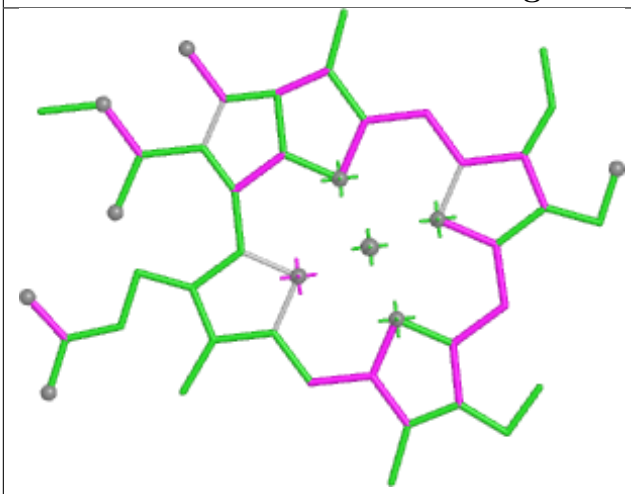


Torsions

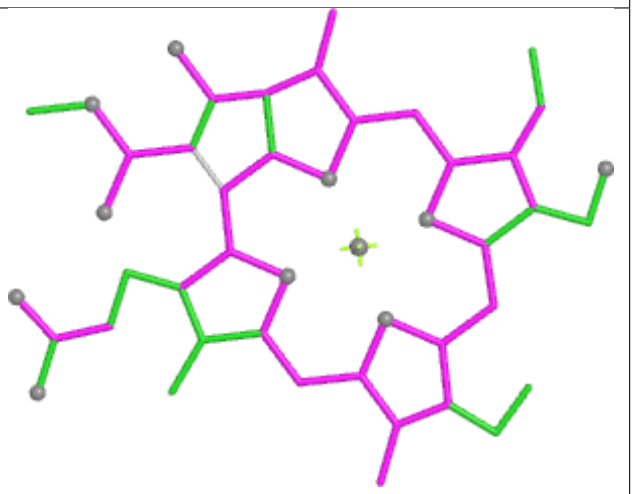


Rings

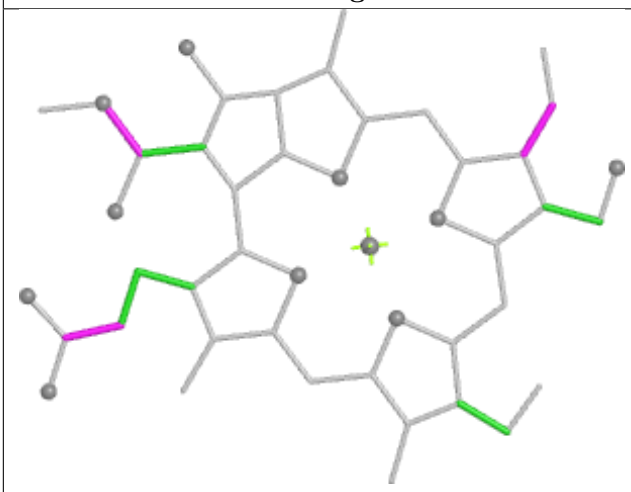
Ligand CHL R 608



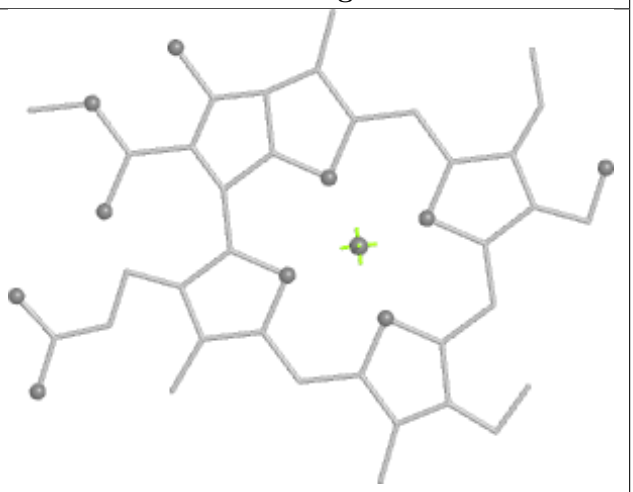
Bond lengths



Bond angles

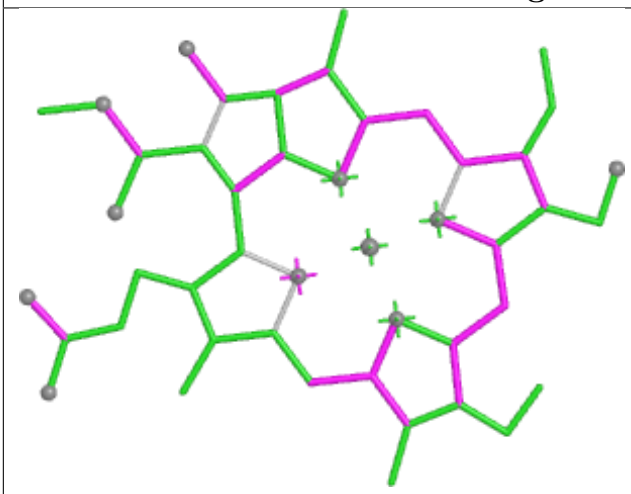


Torsions

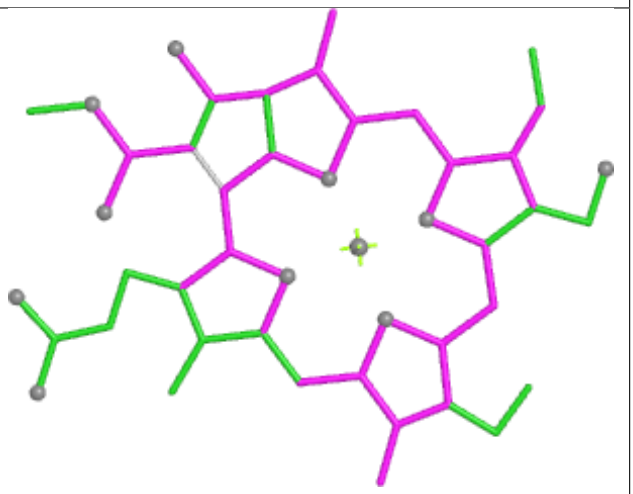


Rings

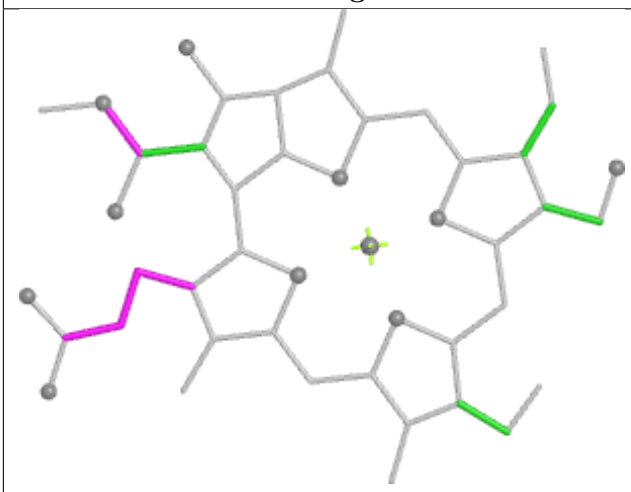
Ligand CHL 6 310



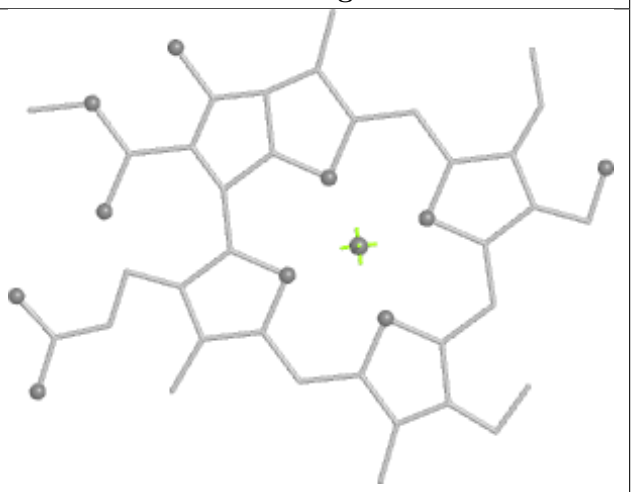
Bond lengths



Bond angles

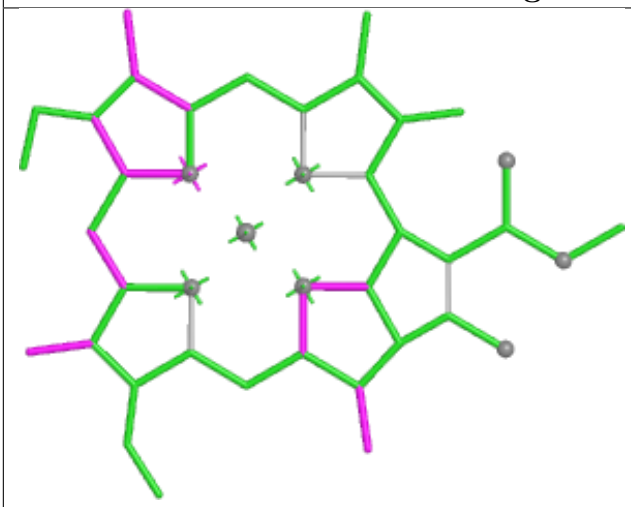


Torsions

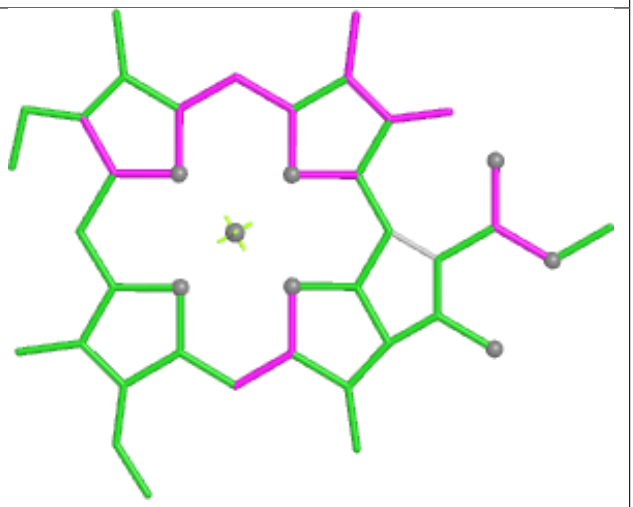


Rings

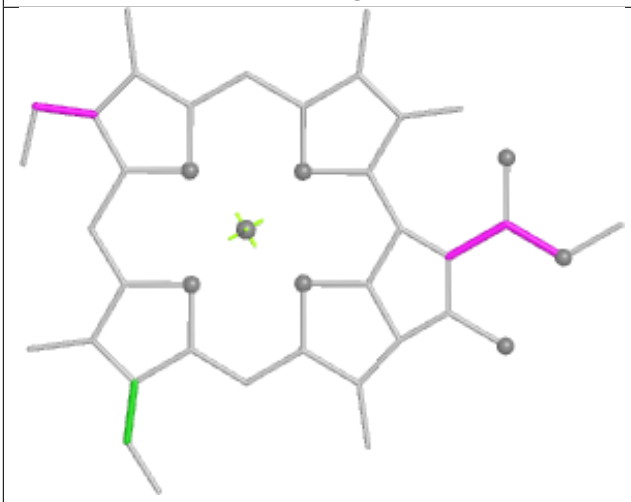
Ligand CLA R 604



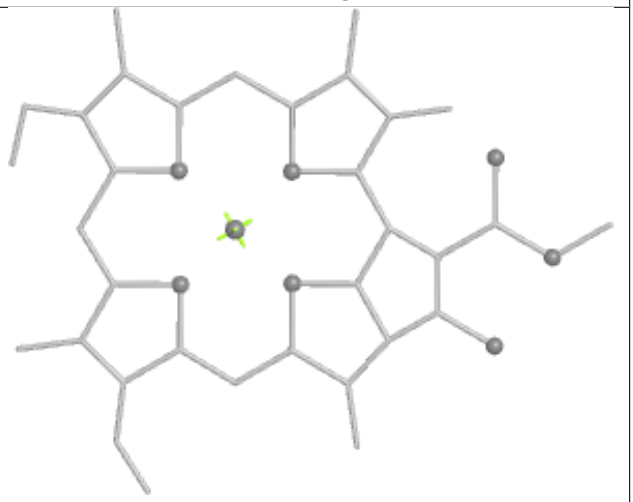
Bond lengths



Bond angles

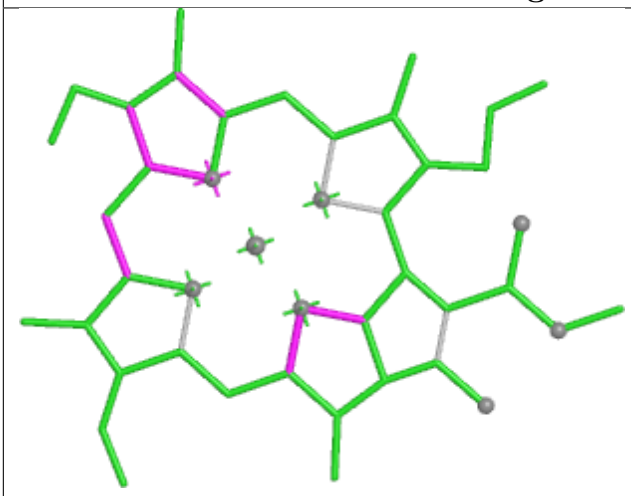


Torsions

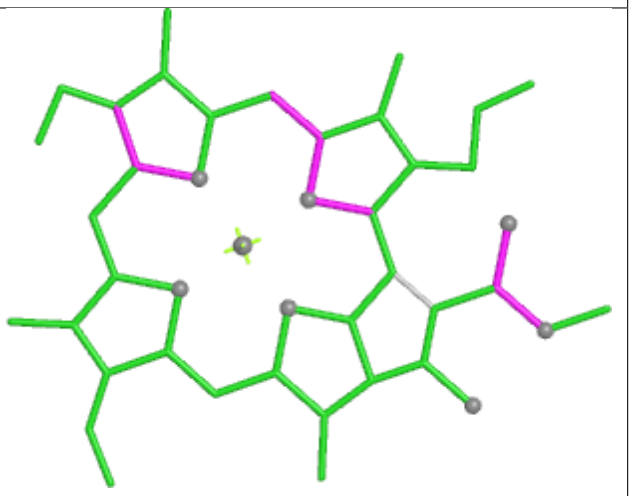


Rings

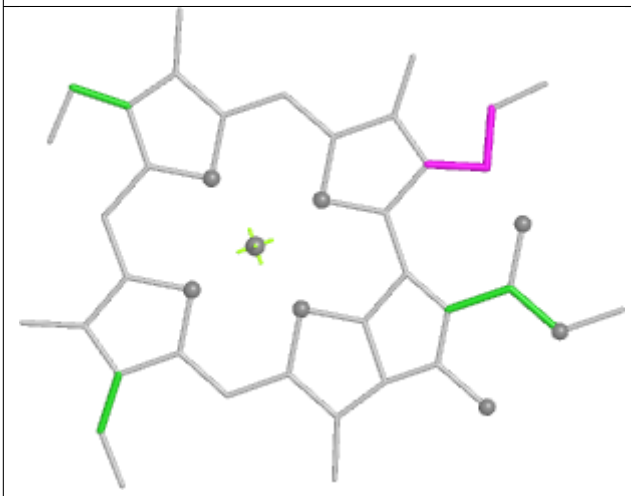
Ligand CLA n 316



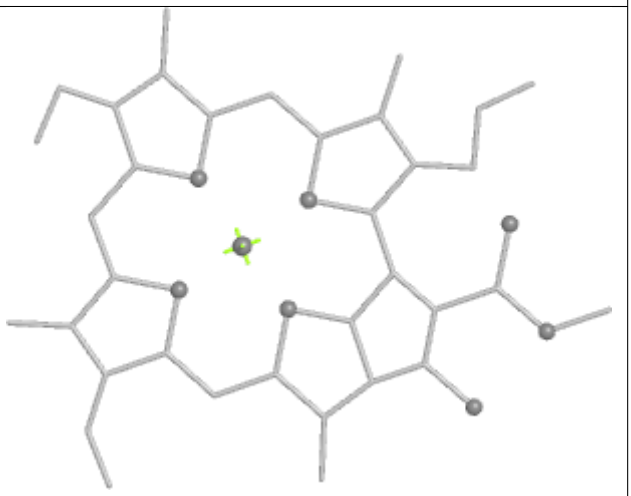
Bond lengths



Bond angles

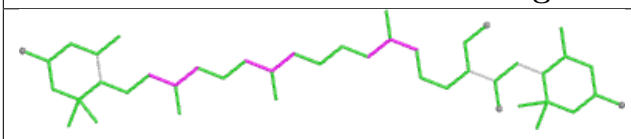


Torsions

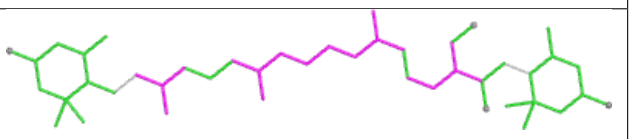


Rings

Ligand 0IE N 302



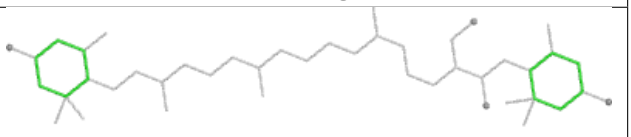
Bond lengths



Bond angles

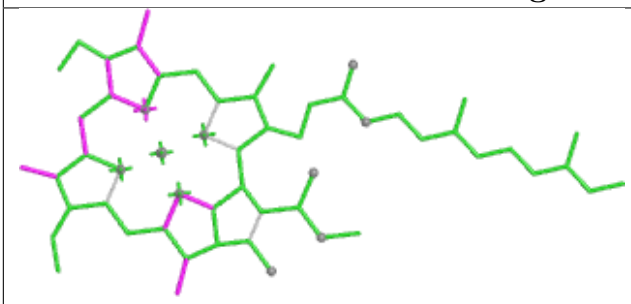


Torsions

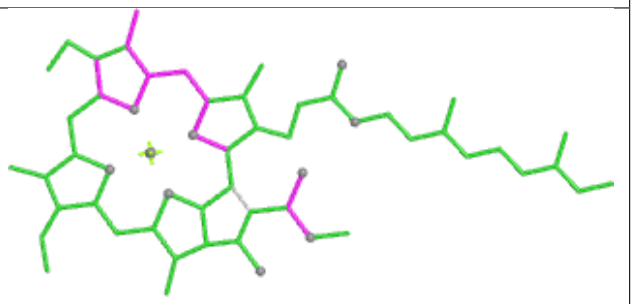


Rings

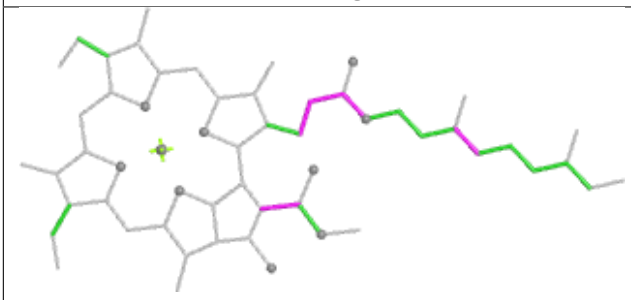
Ligand CLA c 605



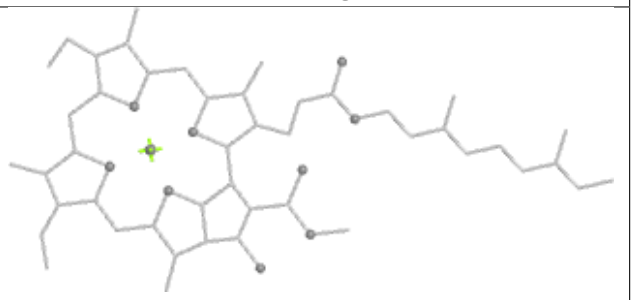
Bond lengths



Bond angles

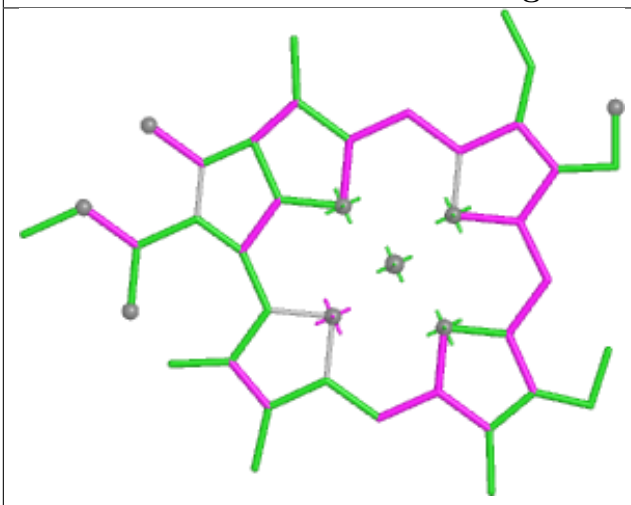


Torsions

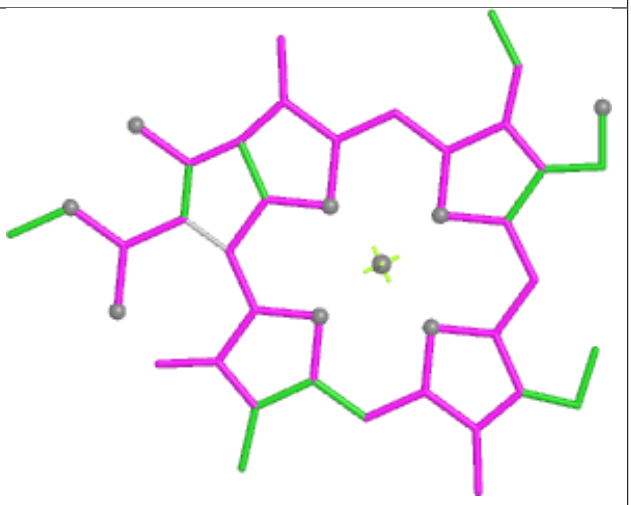


Rings

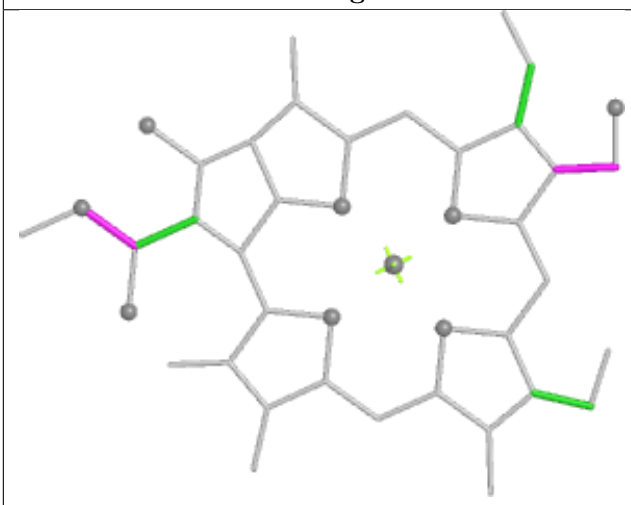
Ligand CHL N 317



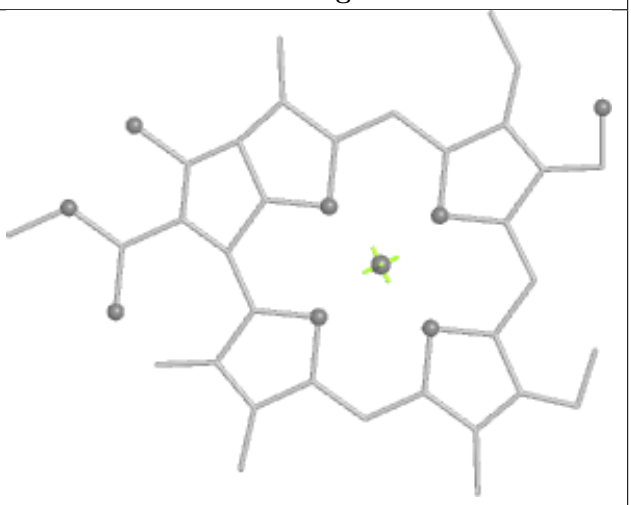
Bond lengths



Bond angles

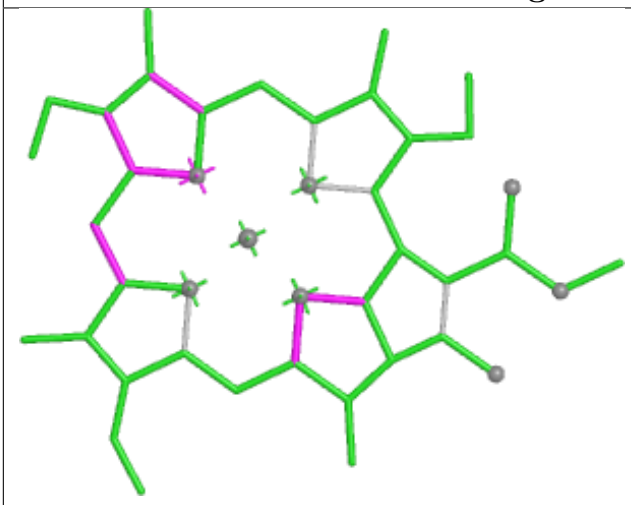


Torsions

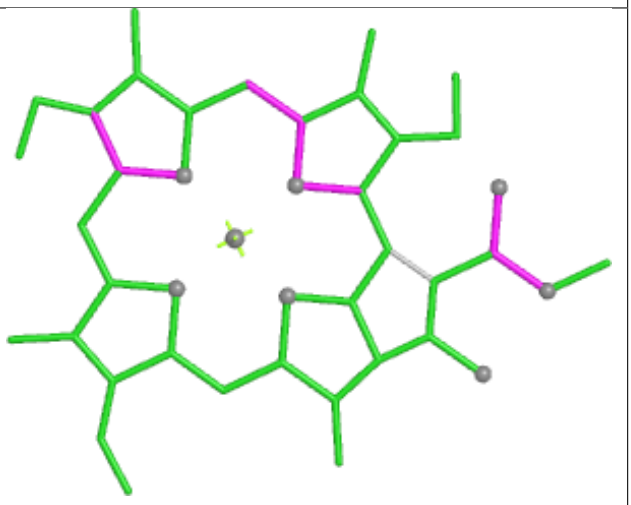


Rings

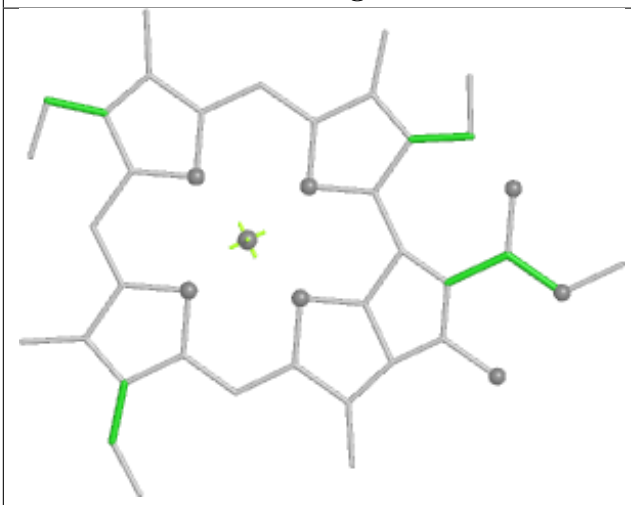
Ligand CLA 4 316



Bond lengths



Bond angles

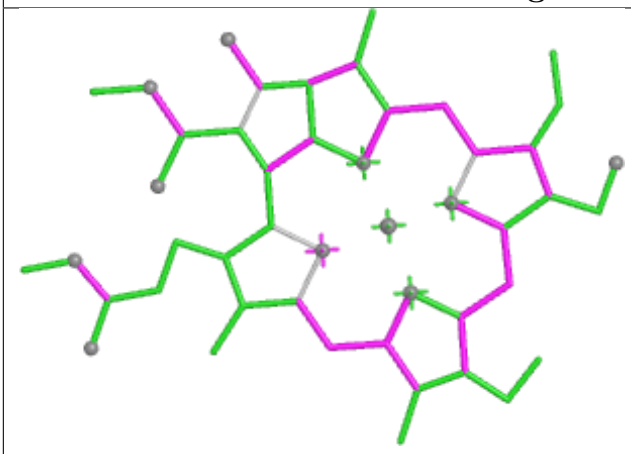


Torsions

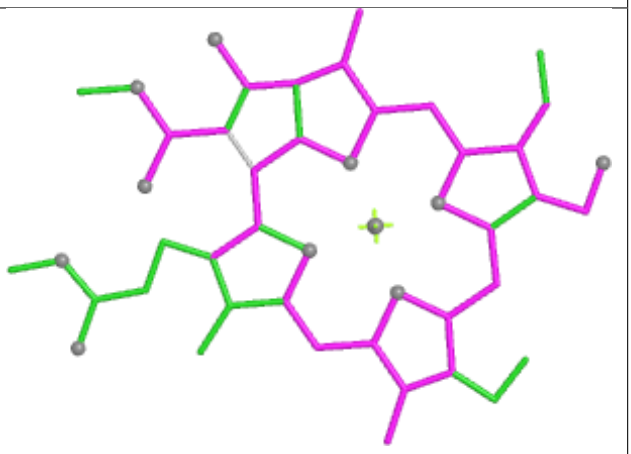


Rings

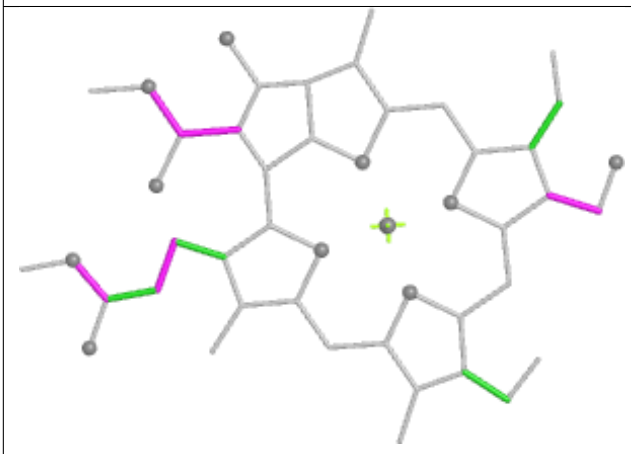
Ligand CHL 5 306



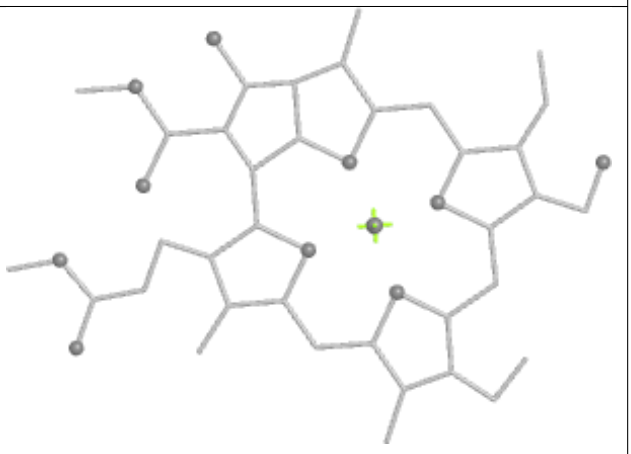
Bond lengths



Bond angles

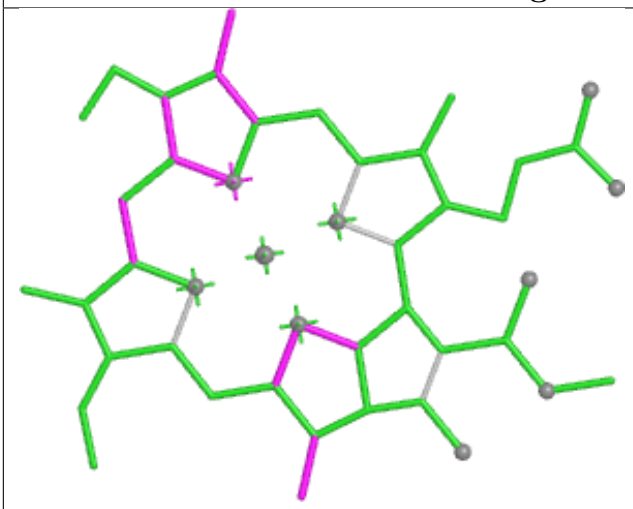


Torsions

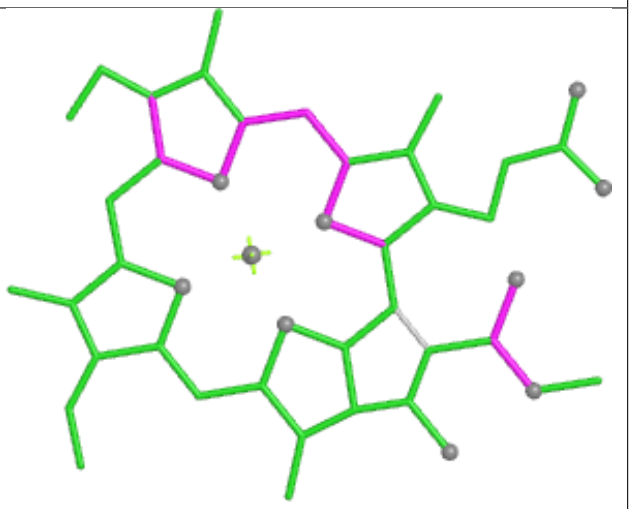


Rings

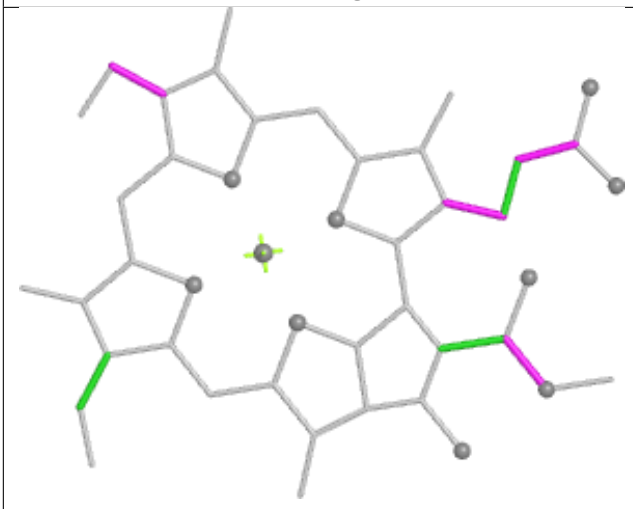
Ligand CLA s 417



Bond lengths



Bond angles

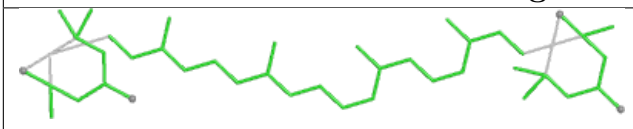


Torsions

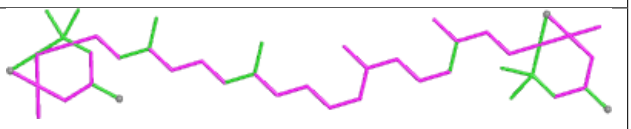


Rings

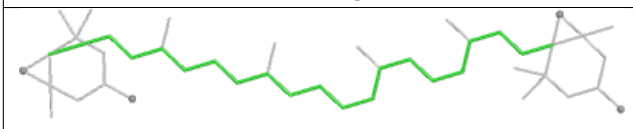
Ligand XAT r 316



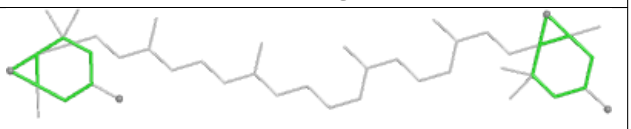
Bond lengths



Bond angles

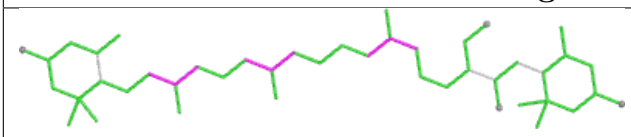


Torsions

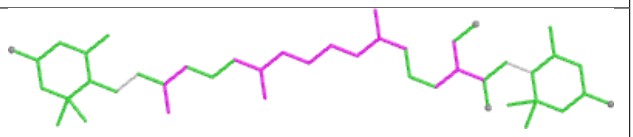


Rings

Ligand 0IE 2 302



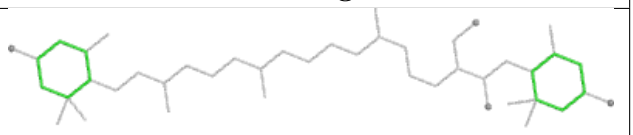
Bond lengths



Bond angles

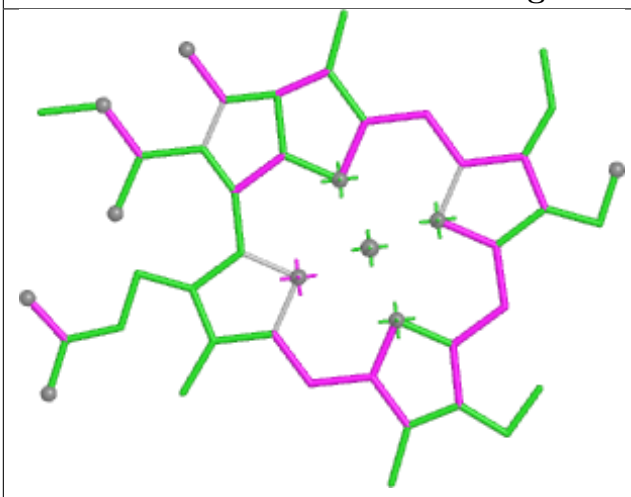


Torsions

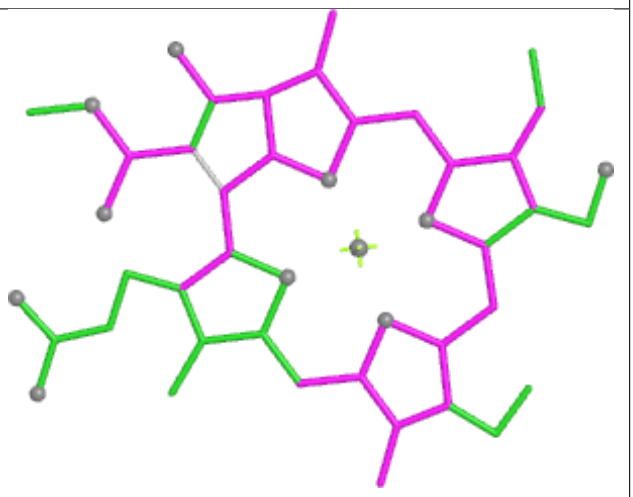


Rings

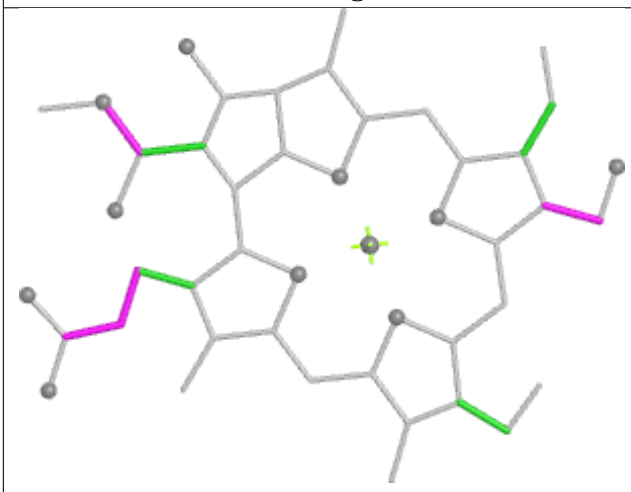
Ligand CHL 5 312



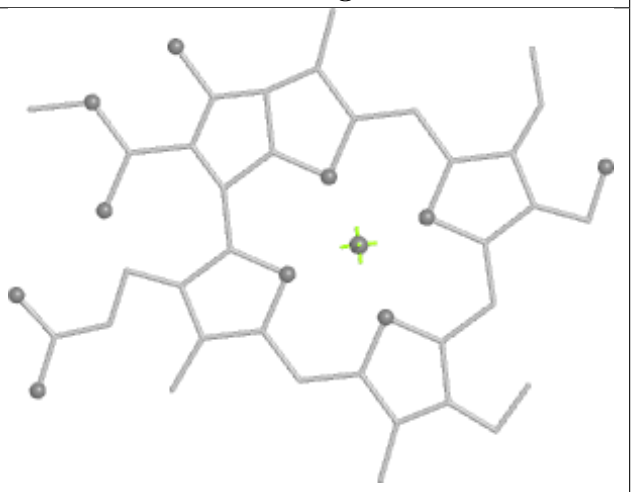
Bond lengths



Bond angles

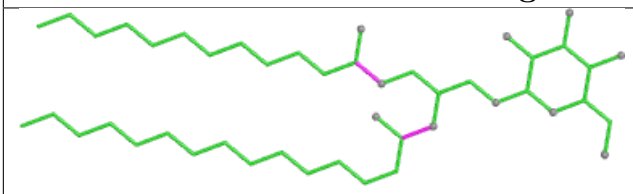


Torsions

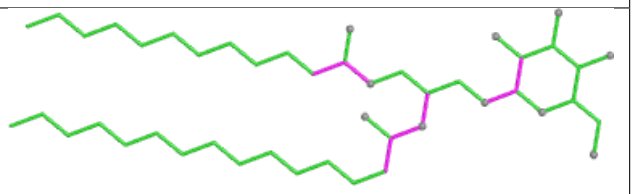


Rings

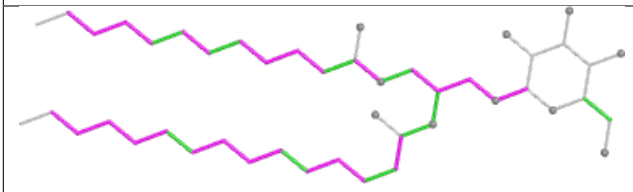
Ligand LMG D 411



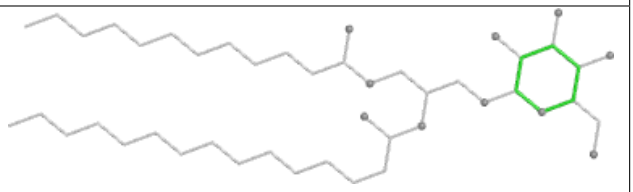
Bond lengths



Bond angles

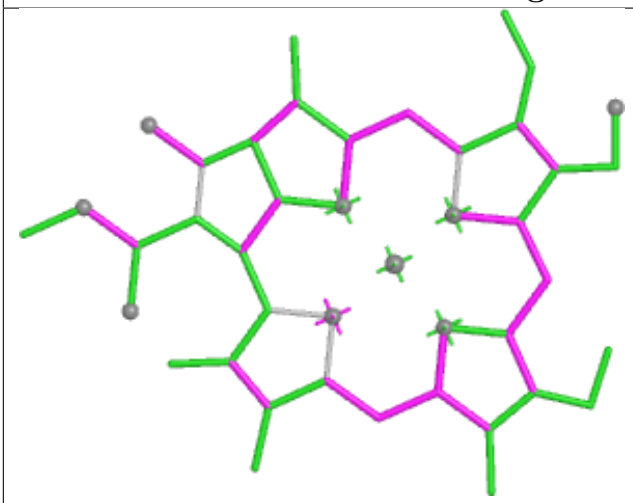


Torsions

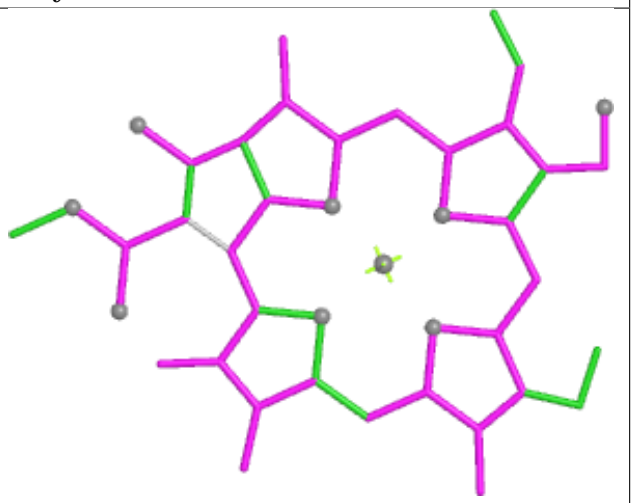


Rings

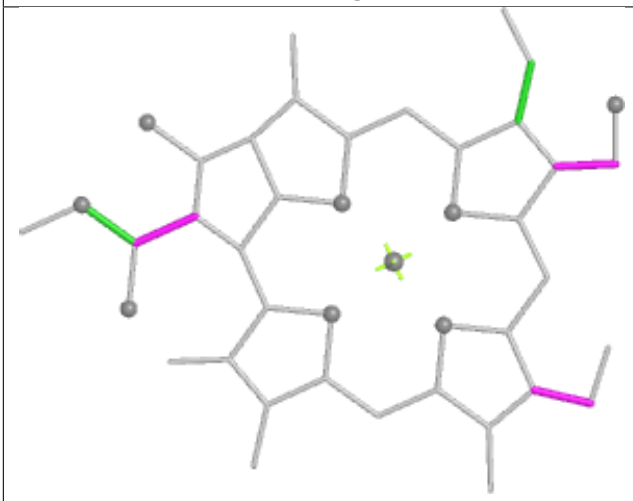
Ligand CHL y 318



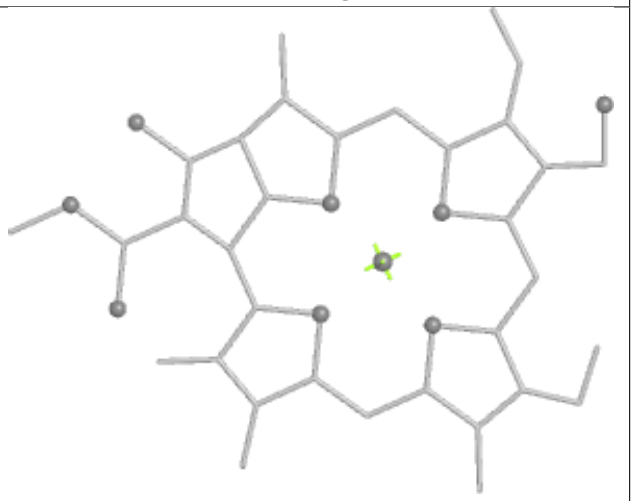
Bond lengths



Bond angles

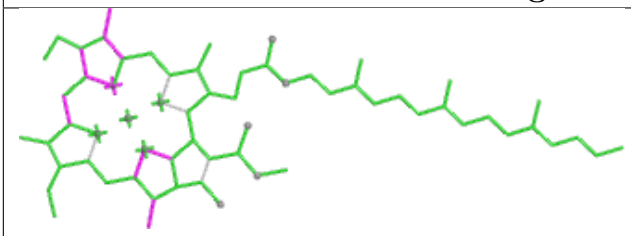


Torsions

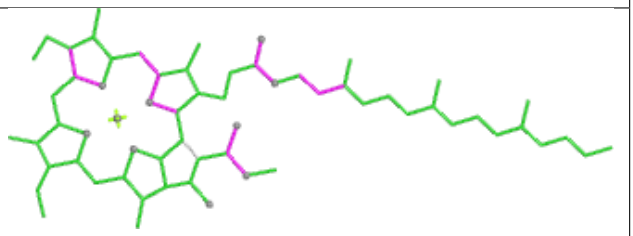


Rings

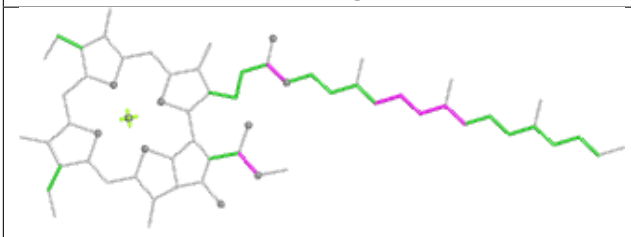
Ligand CLA 8 312



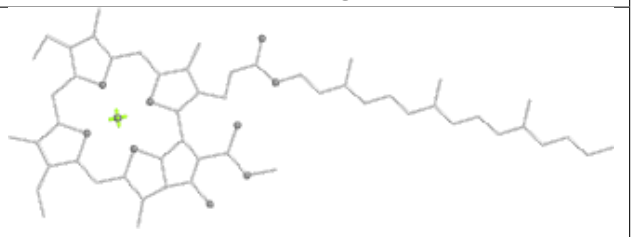
Bond lengths



Bond angles

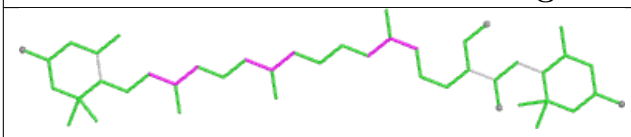


Torsions

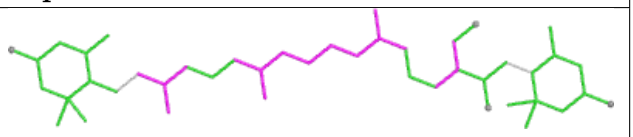


Rings

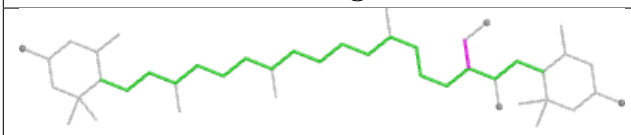
Ligand 0IE p 303



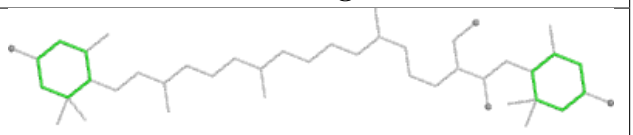
Bond lengths



Bond angles

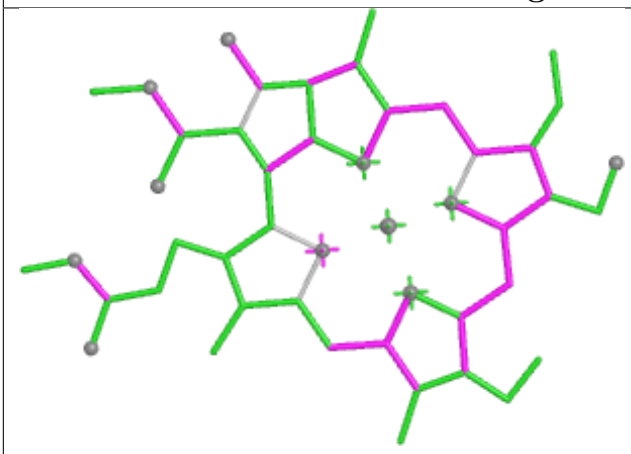


Torsions

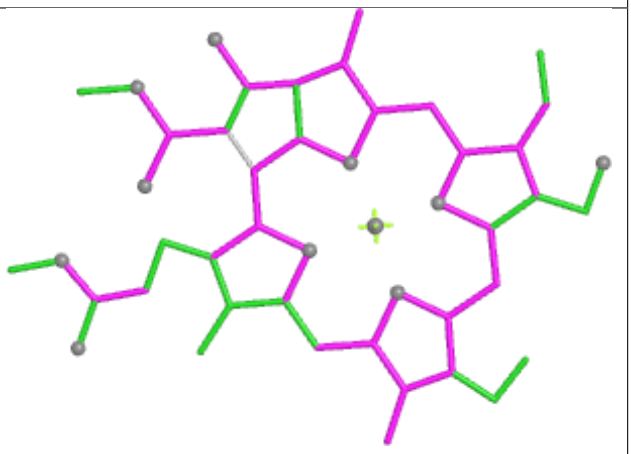


Rings

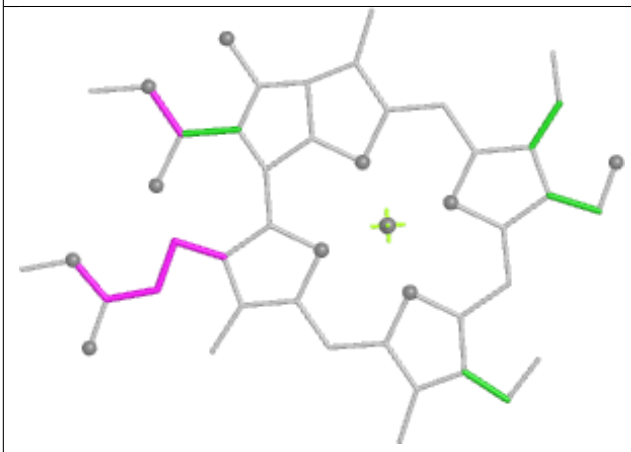
Ligand CHL 2 311



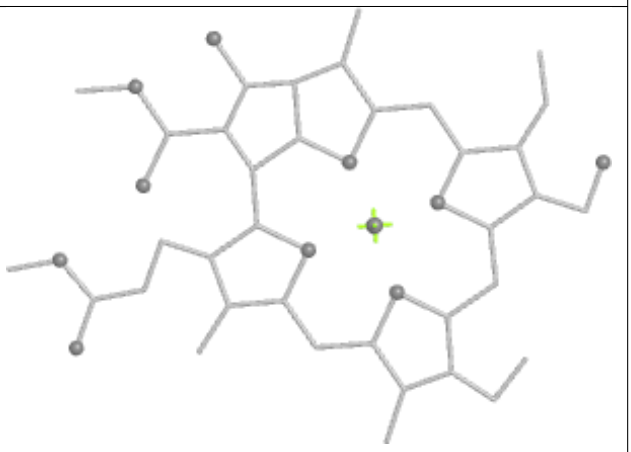
Bond lengths



Bond angles

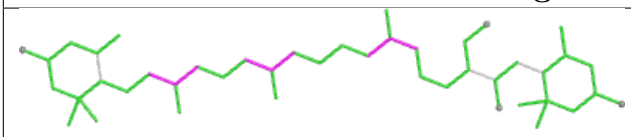


Torsions

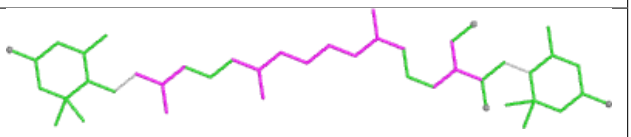


Rings

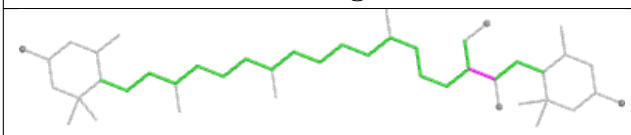
Ligand 0IE Y 302



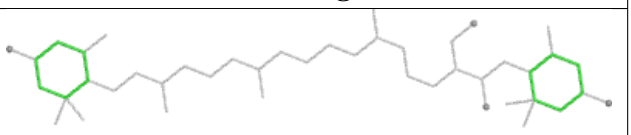
Bond lengths



Bond angles

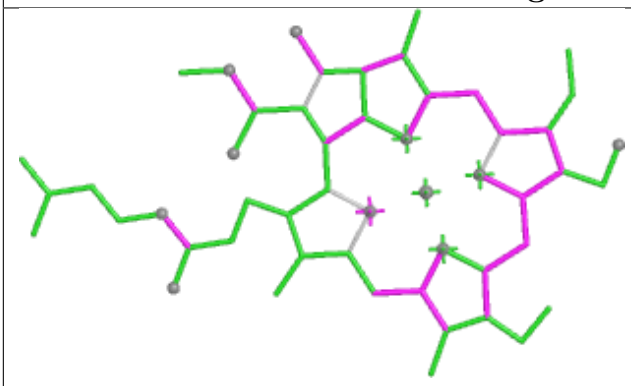


Torsions

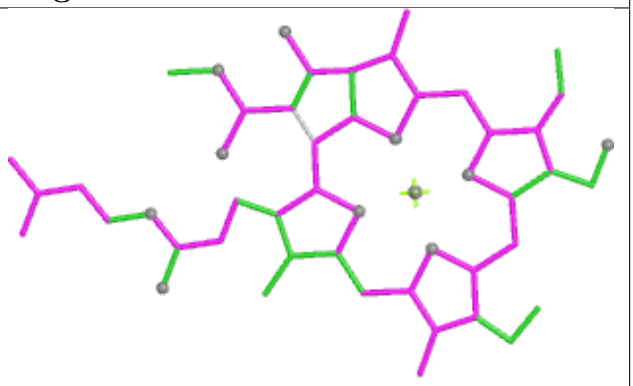


Rings

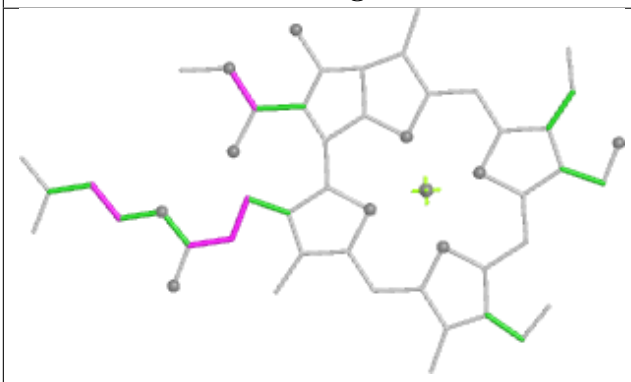
Ligand CHL g 312



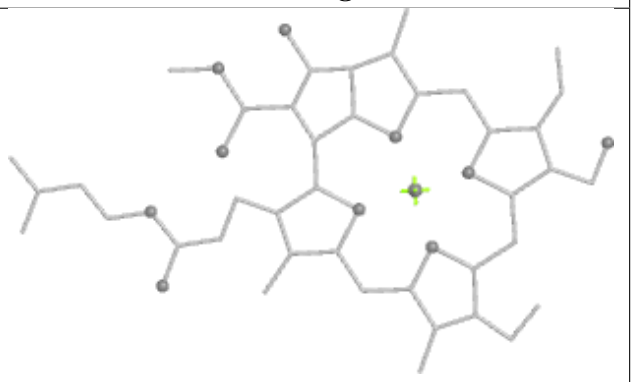
Bond lengths



Bond angles

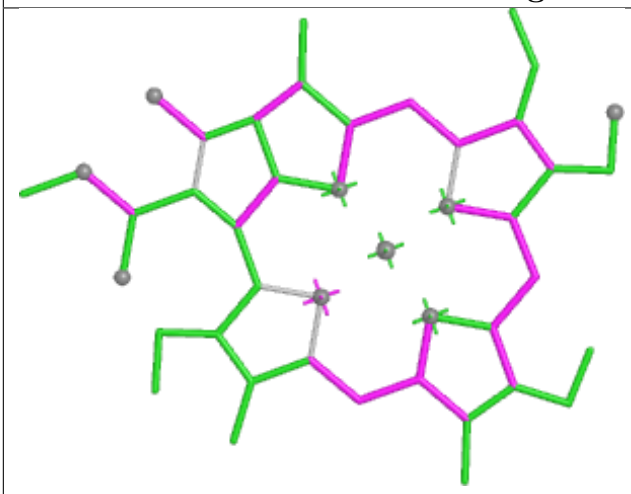


Torsions

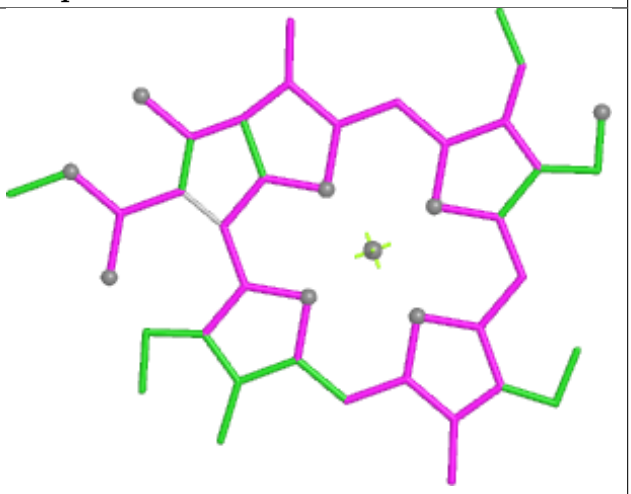


Rings

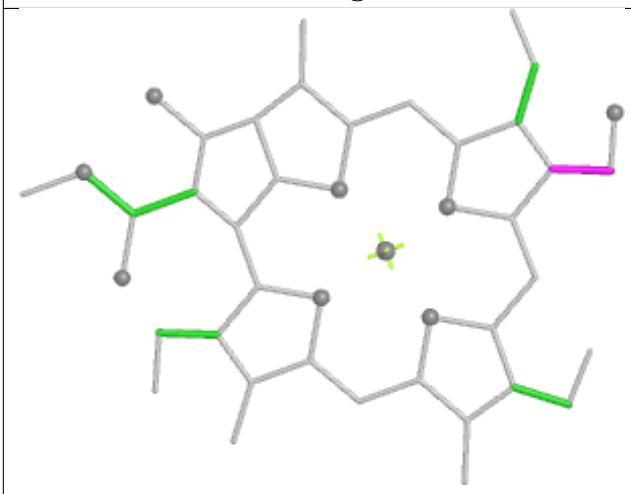
Ligand CHL q 307



Bond lengths



Bond angles



Torsions

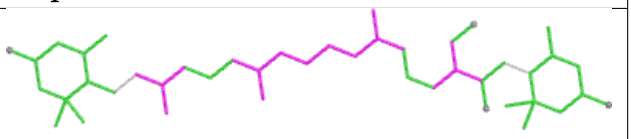


Rings

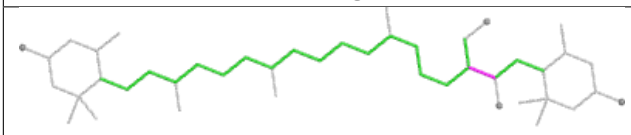
Ligand 0IE q 302



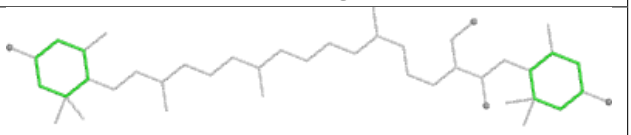
Bond lengths



Bond angles

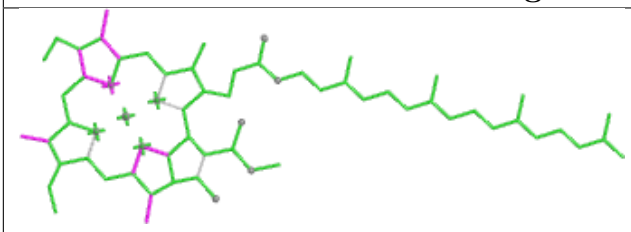


Torsions

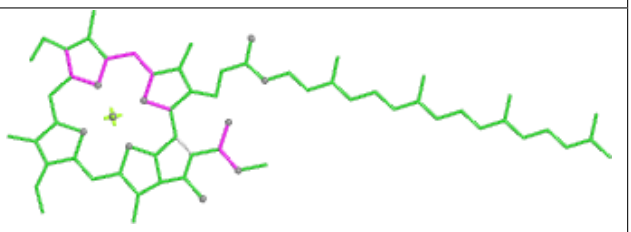


Rings

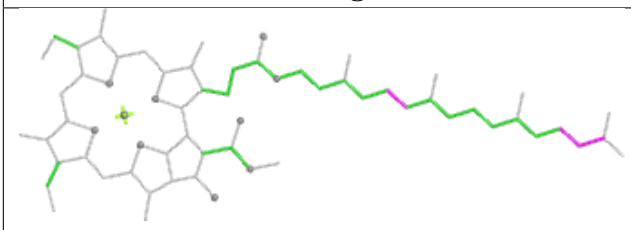
Ligand CLA B 615



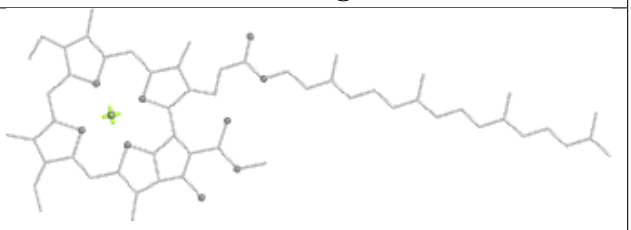
Bond lengths



Bond angles

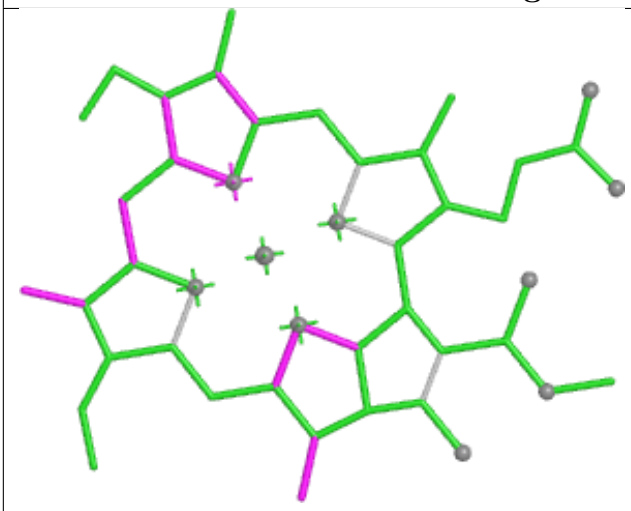


Torsions

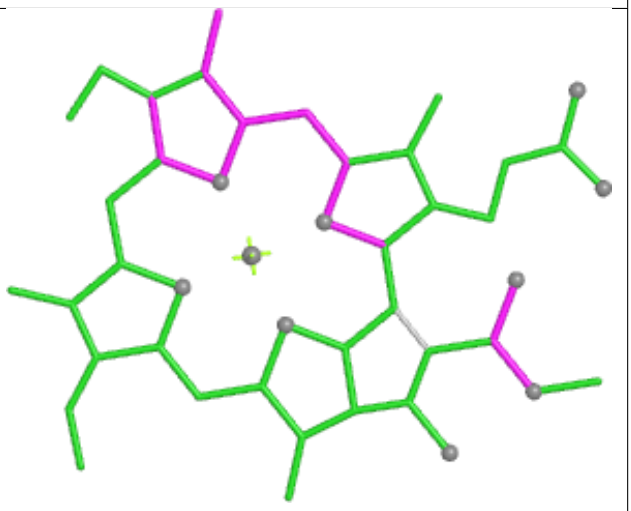


Rings

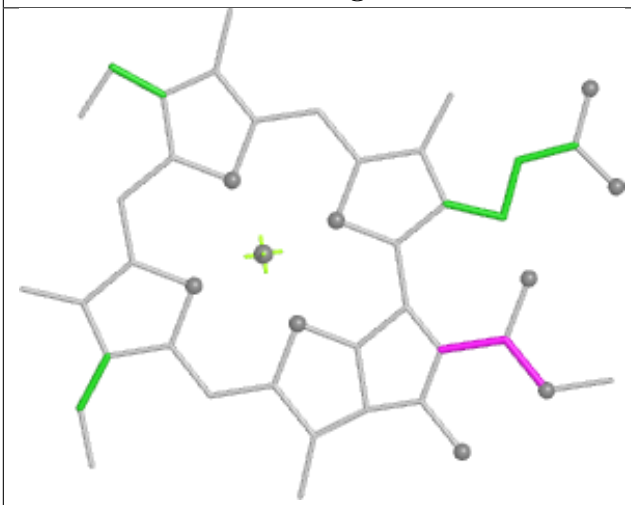
Ligand CLA R 610



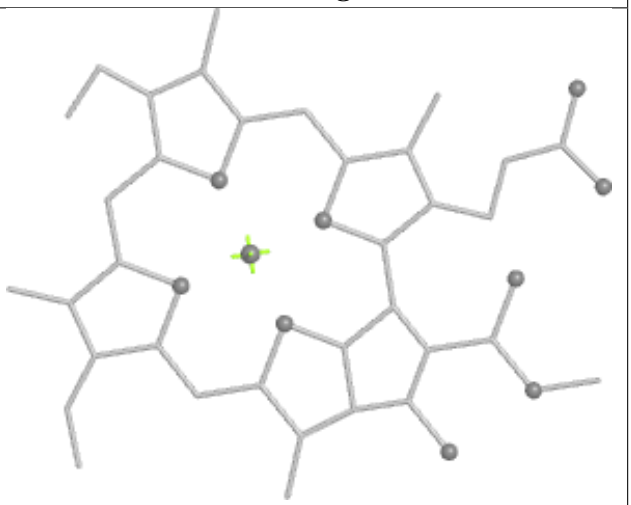
Bond lengths



Bond angles

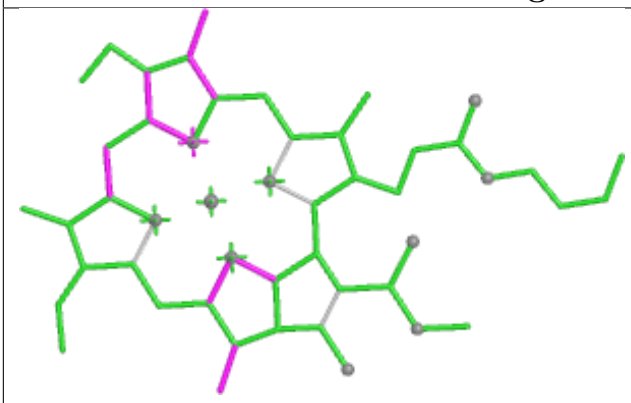


Torsions

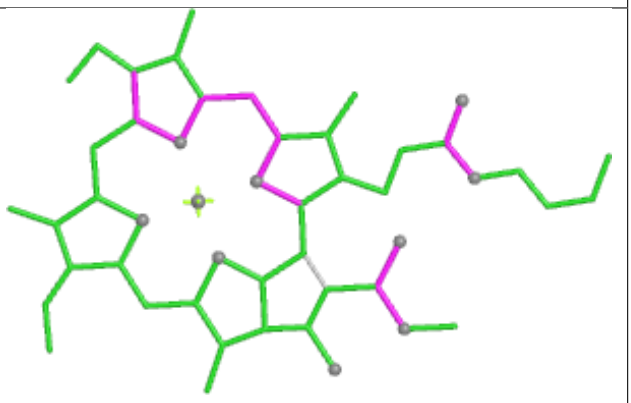


Rings

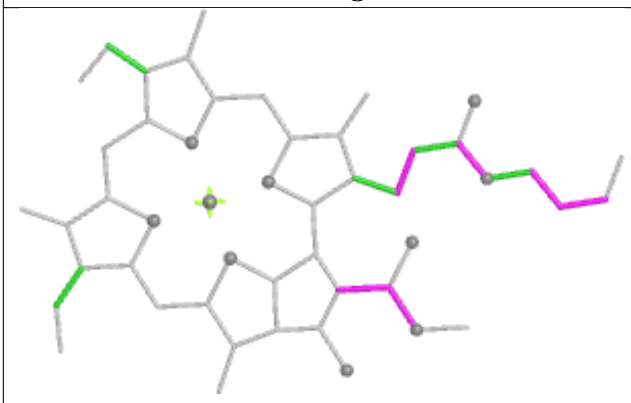
Ligand CLA 5 317



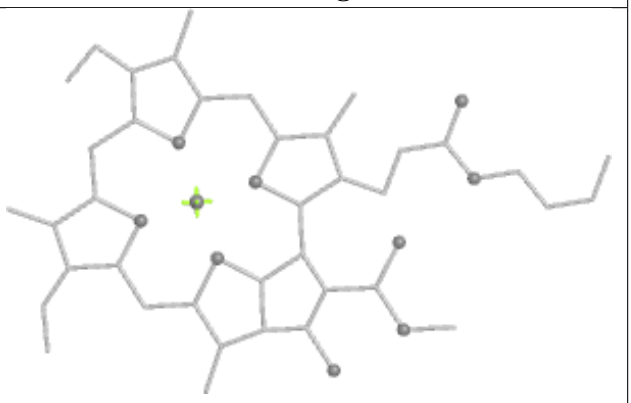
Bond lengths



Bond angles

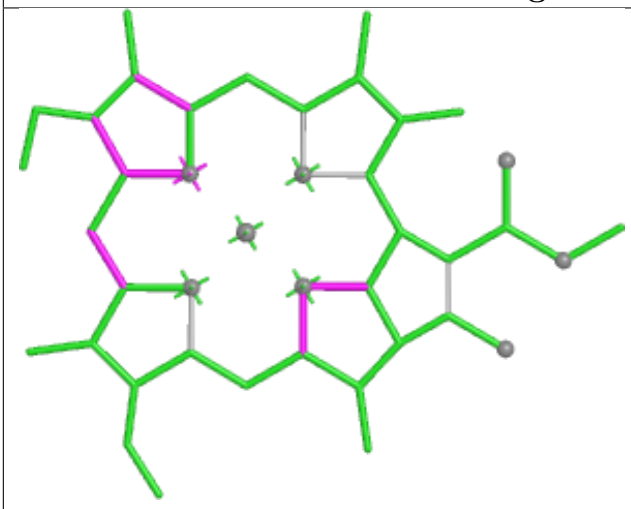


Torsions

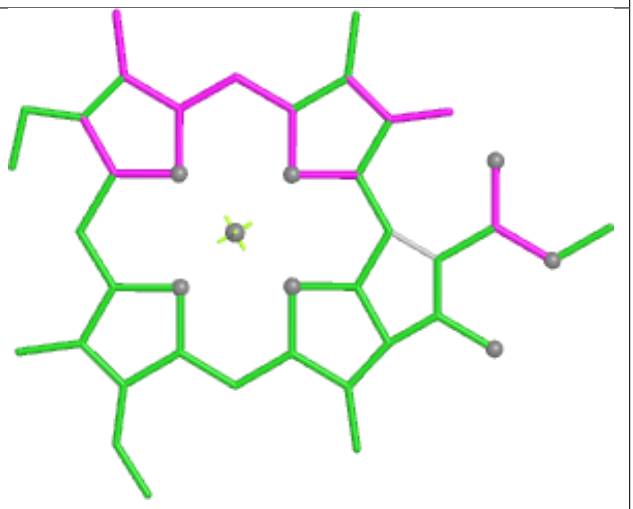


Rings

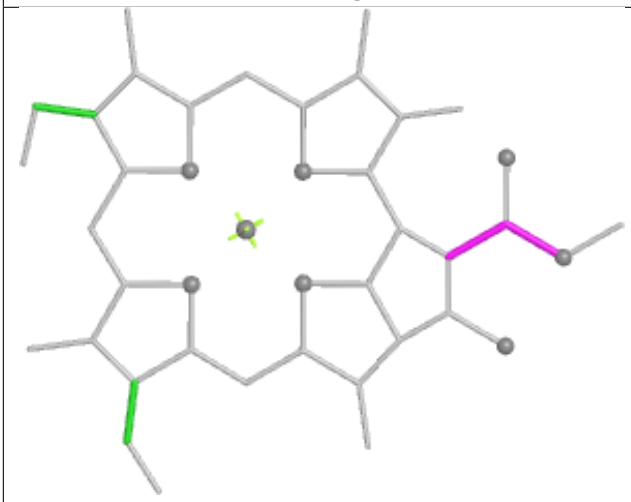
Ligand CLA 3 314



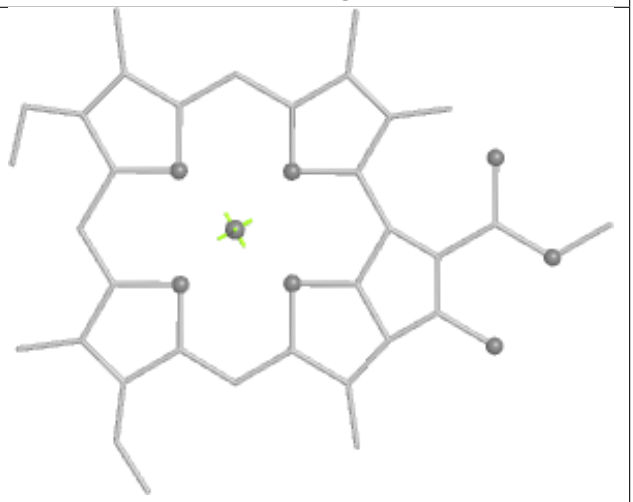
Bond lengths



Bond angles

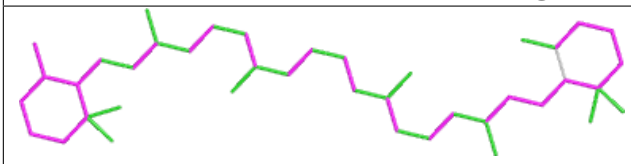


Torsions

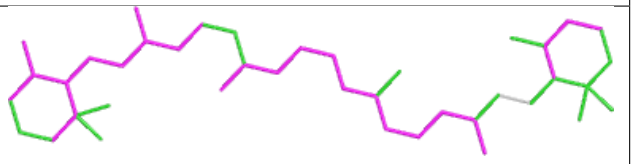


Rings

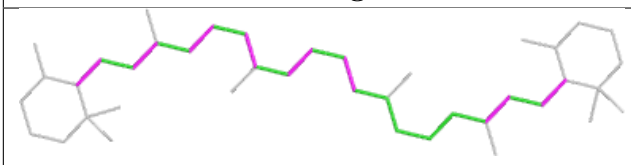
Ligand 8CT t 101



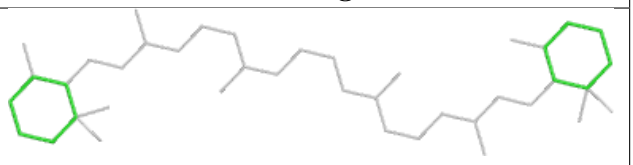
Bond lengths



Bond angles

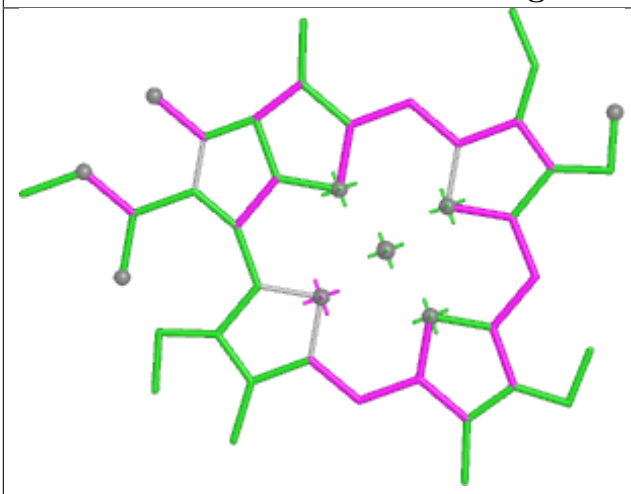


Torsions

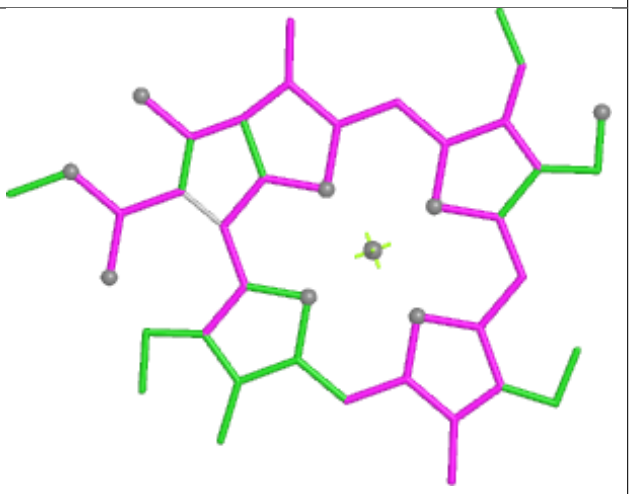


Rings

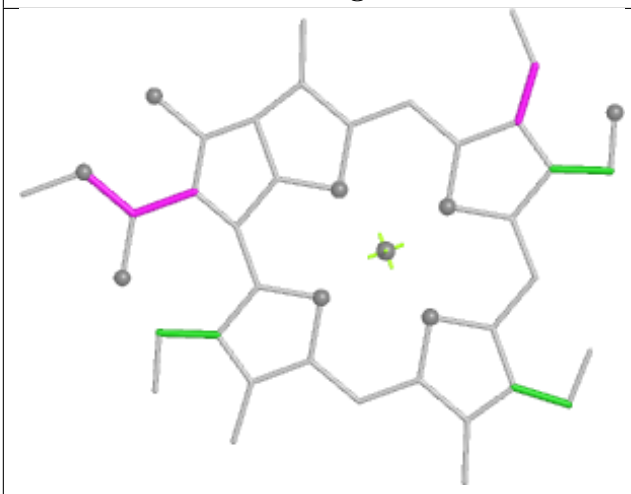
Ligand CHL 7 313



Bond lengths



Bond angles

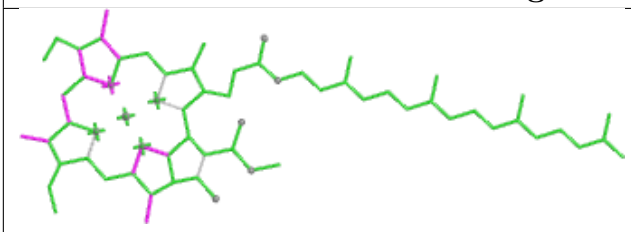


Torsions

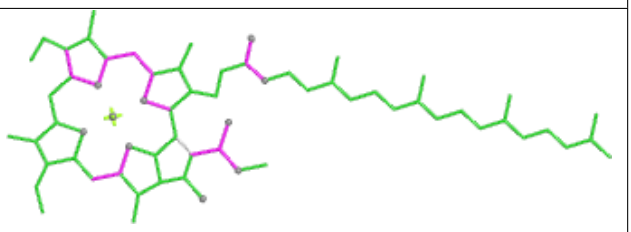


Rings

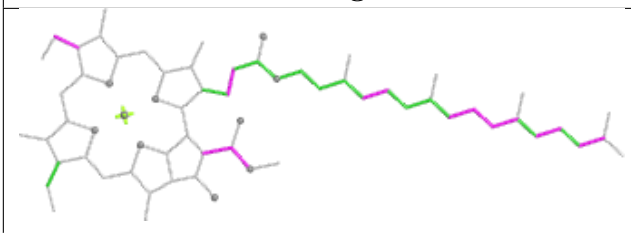
Ligand CLA b 607



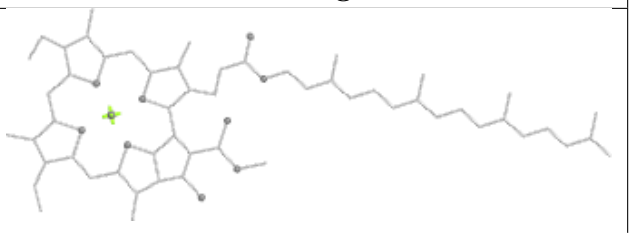
Bond lengths



Bond angles

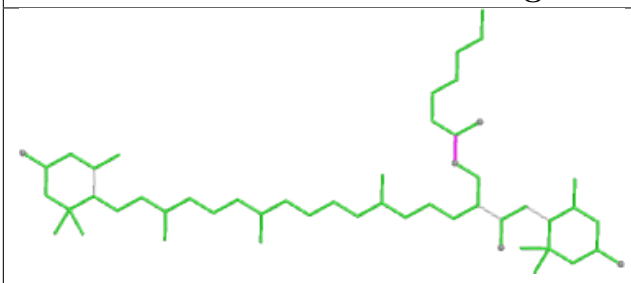


Torsions

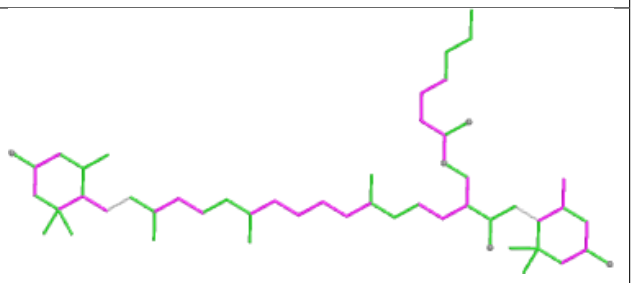


Rings

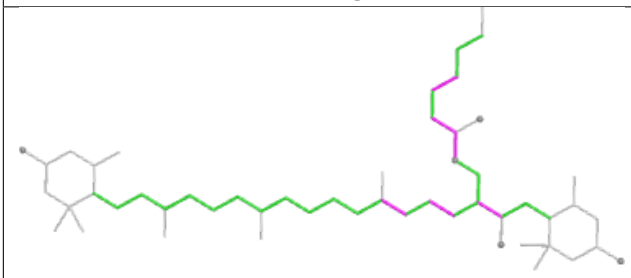
Ligand 0UR N 301



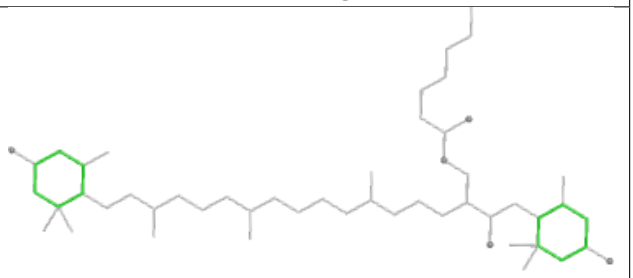
Bond lengths



Bond angles

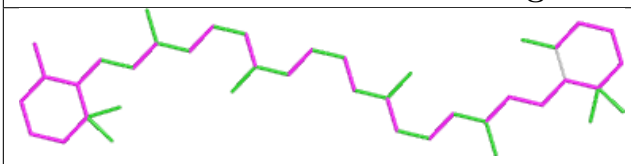


Torsions

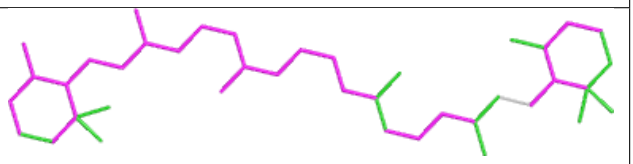


Rings

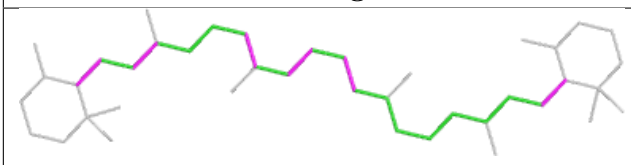
Ligand 8CT C 613



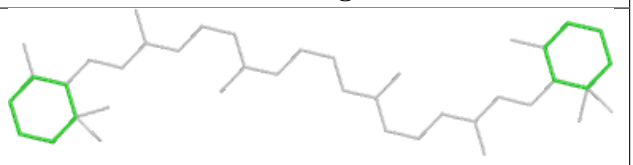
Bond lengths



Bond angles

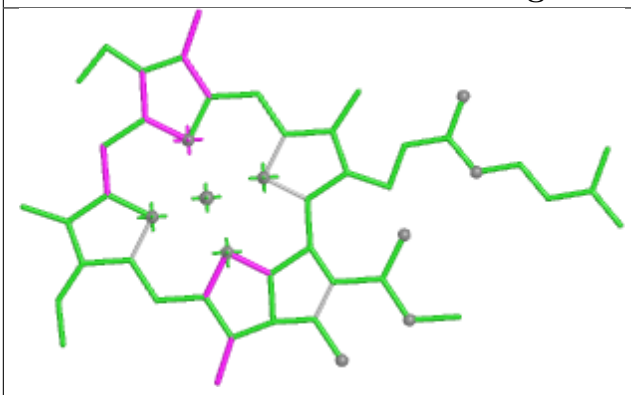


Torsions

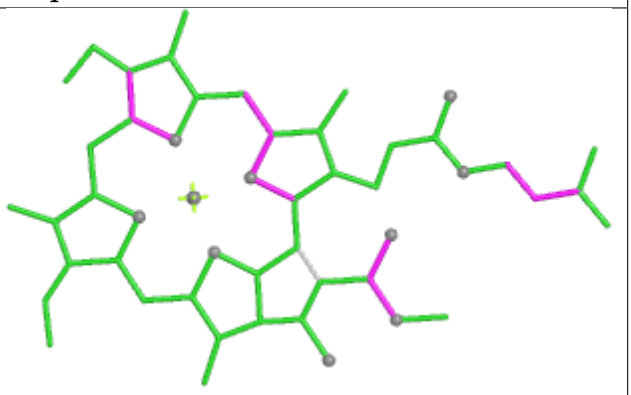


Rings

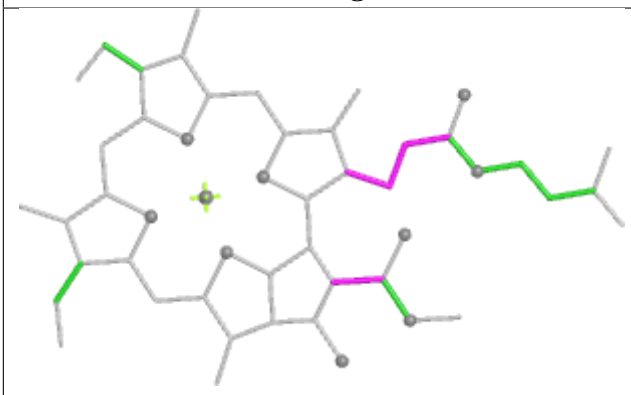
Ligand CLA p 308



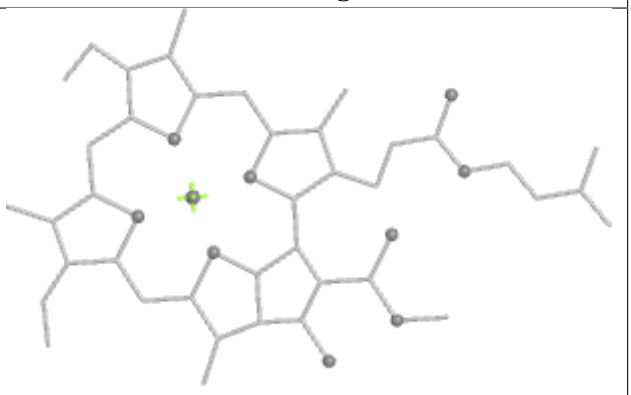
Bond lengths



Bond angles

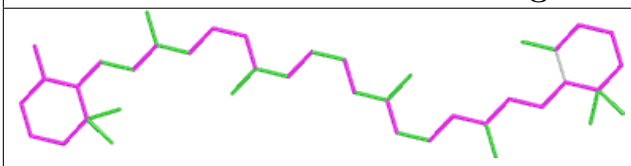


Torsions

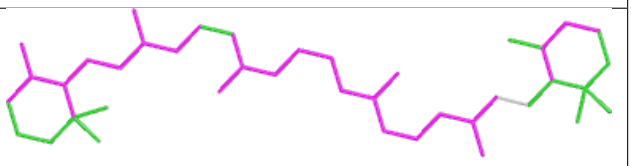


Rings

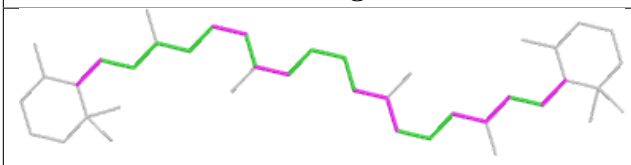
Ligand 8CT S 615



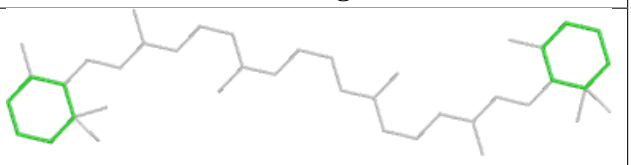
Bond lengths



Bond angles

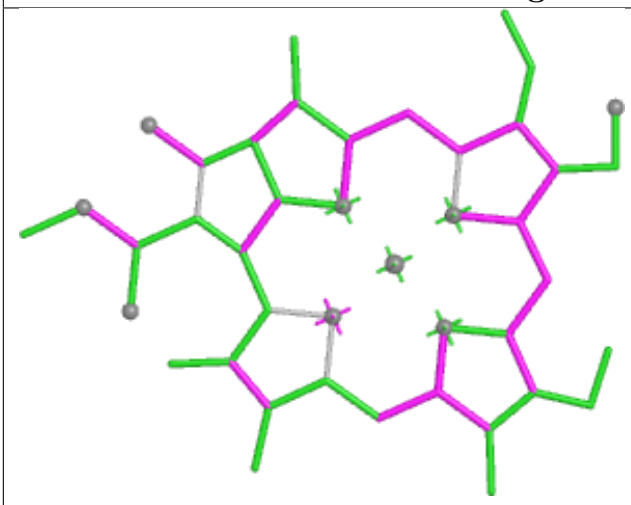


Torsions

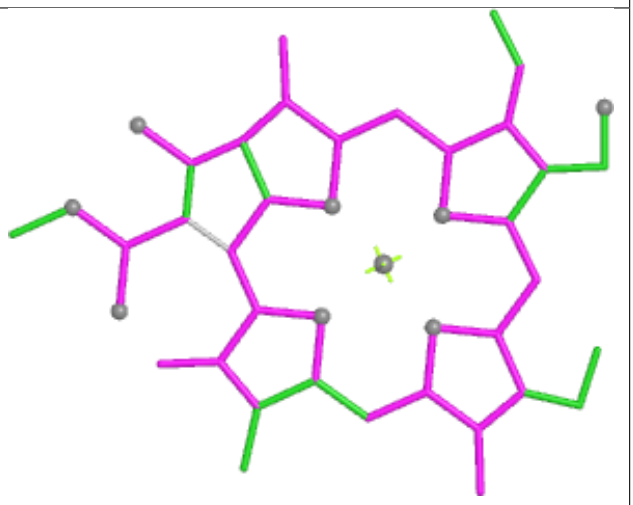


Rings

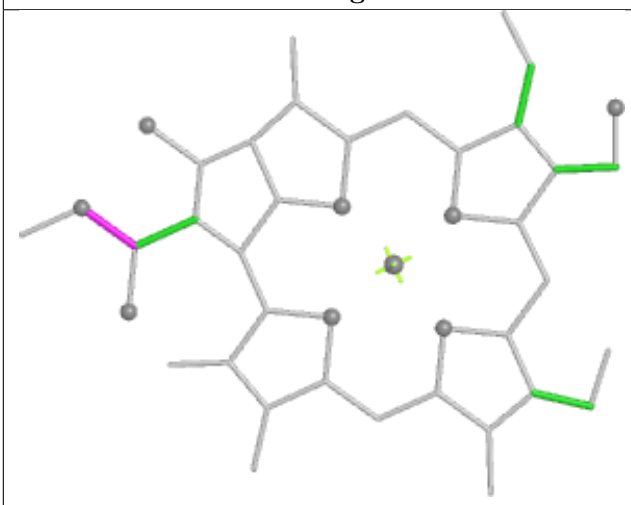
Ligand CHL 4 304



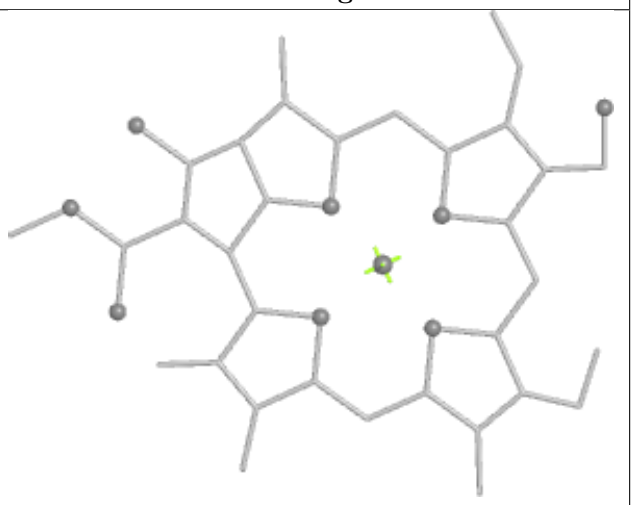
Bond lengths



Bond angles

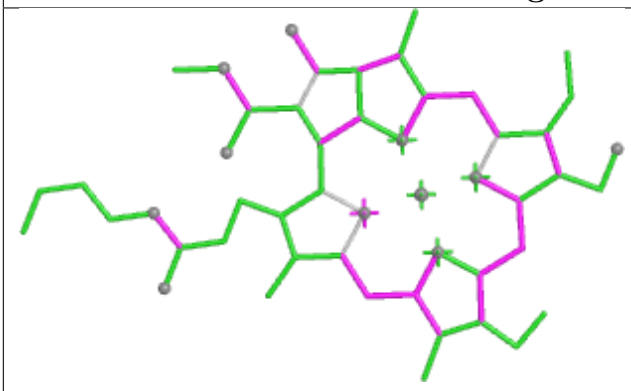


Torsions

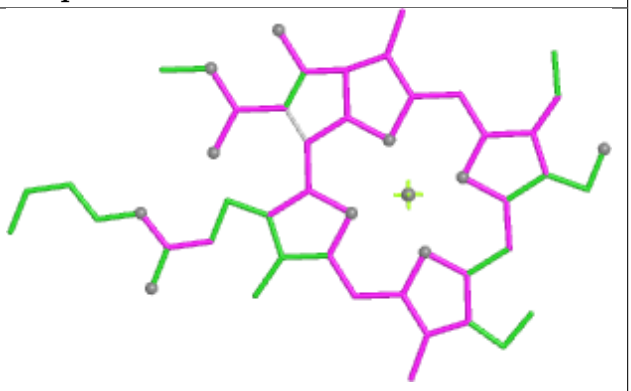


Rings

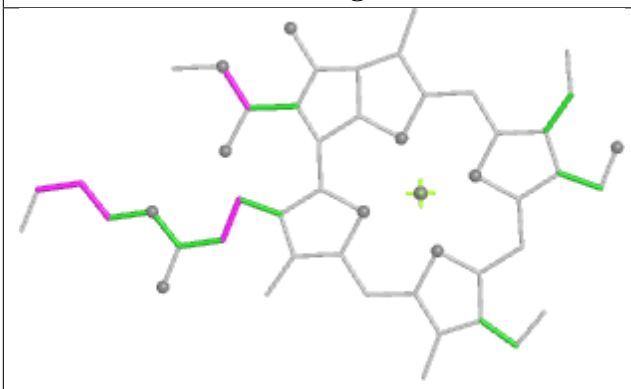
Ligand CHL q 310



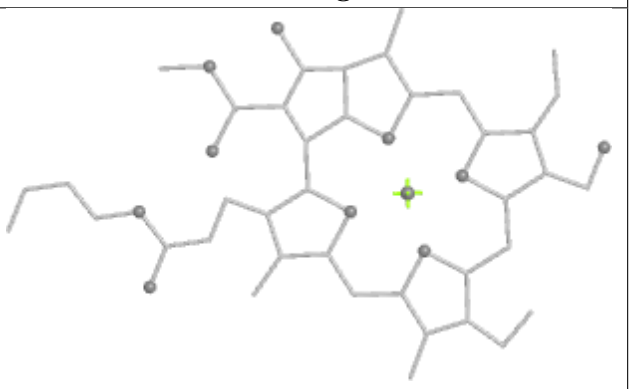
Bond lengths



Bond angles

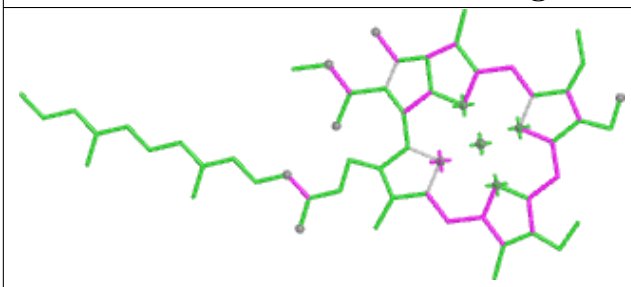


Torsions

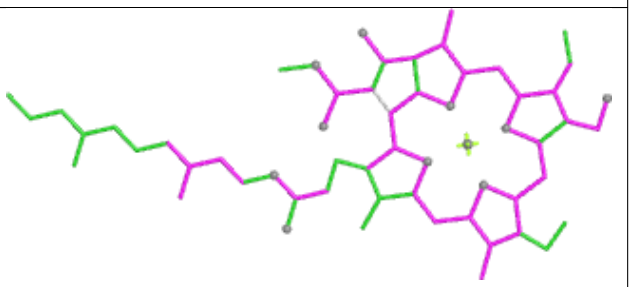


Rings

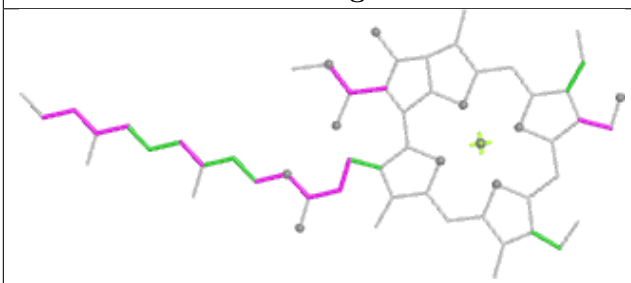
Ligand CHL s 403



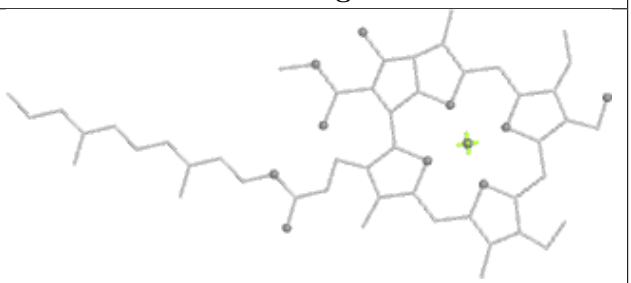
Bond lengths



Bond angles

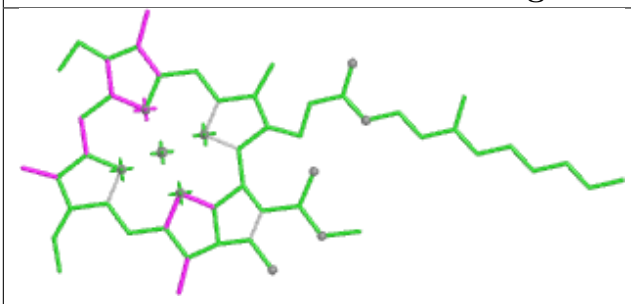


Torsions

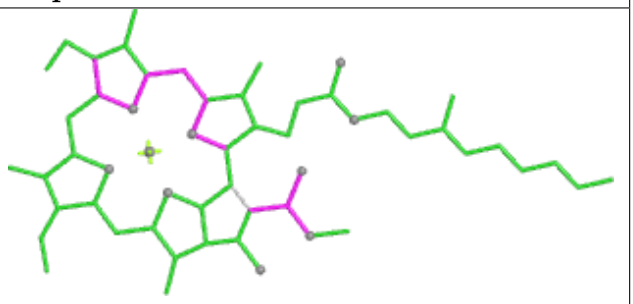


Rings

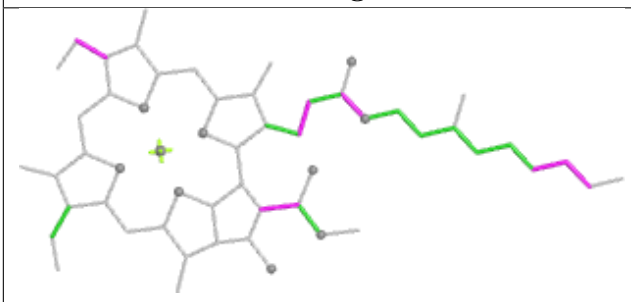
Ligand CLA p 317



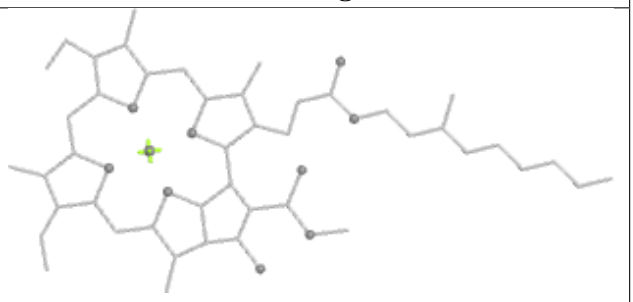
Bond lengths



Bond angles

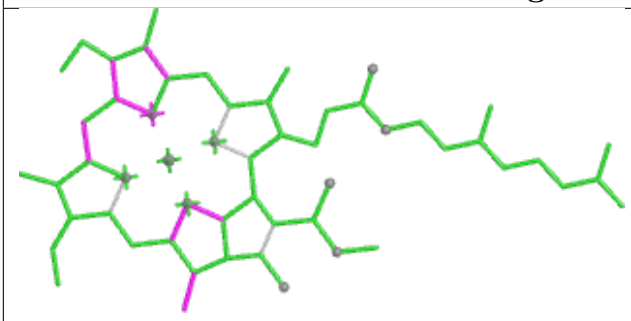


Torsions

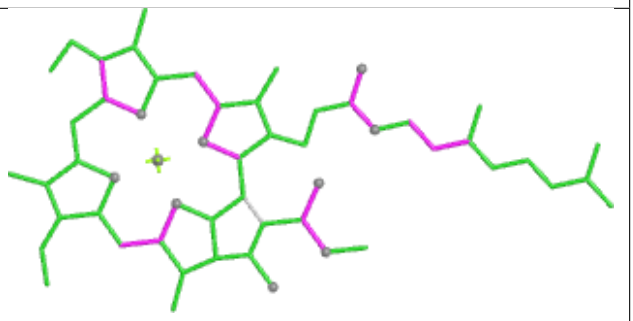


Rings

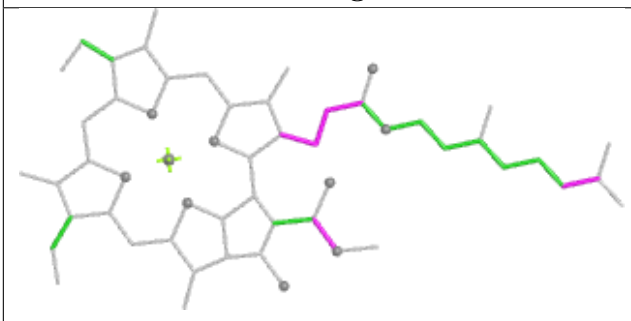
Ligand CLA n 313



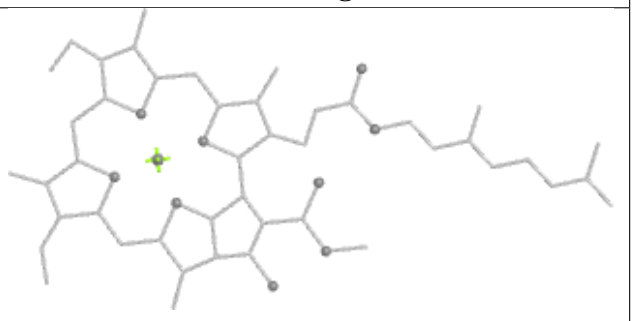
Bond lengths



Bond angles

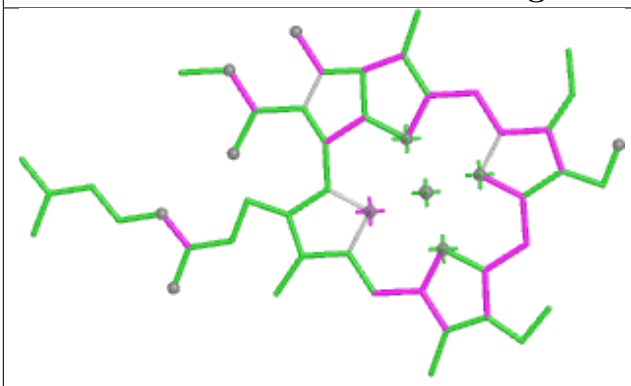


Torsions

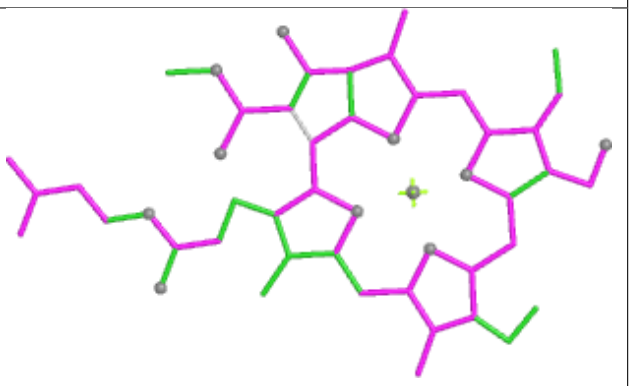


Rings

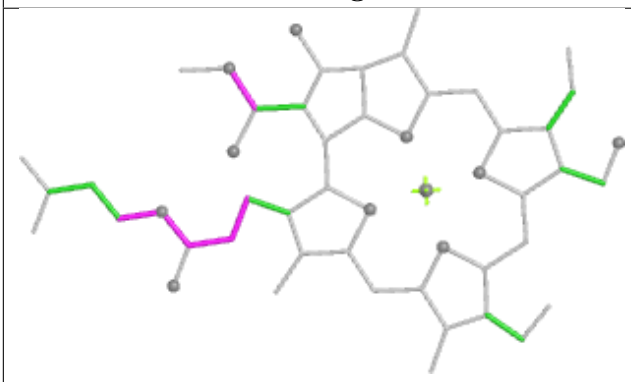
Ligand CHL 3 309



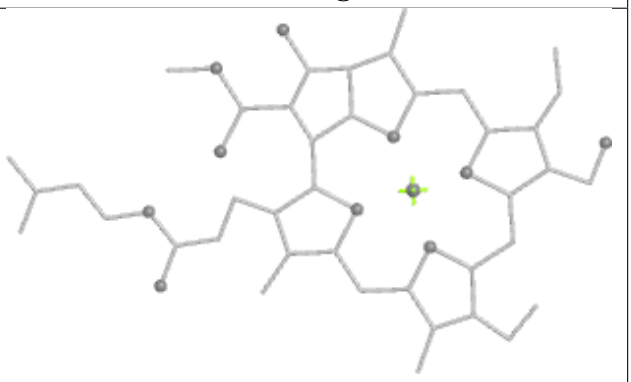
Bond lengths



Bond angles

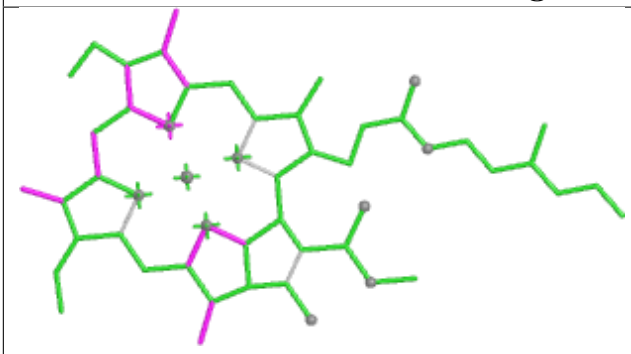


Torsions

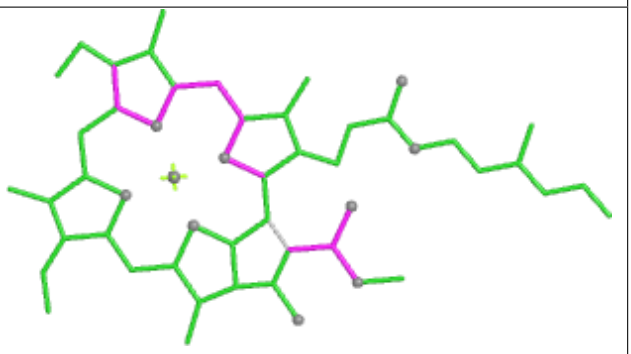


Rings

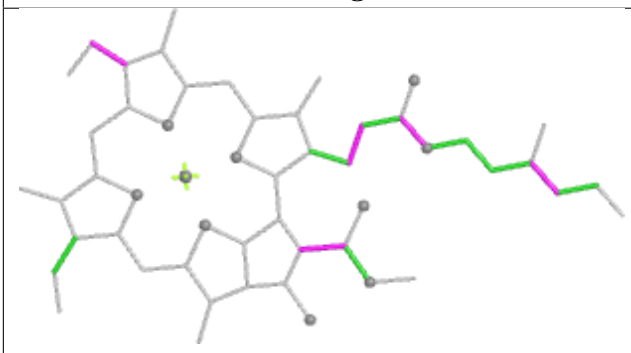
Ligand CLA 7 317



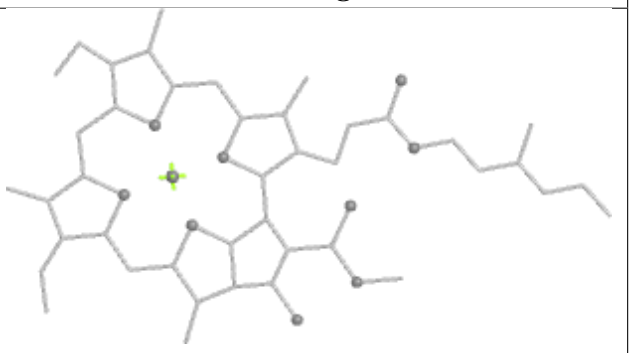
Bond lengths



Bond angles

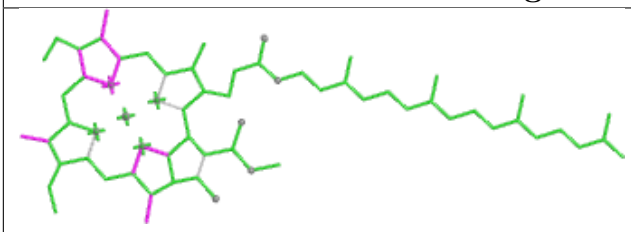


Torsions

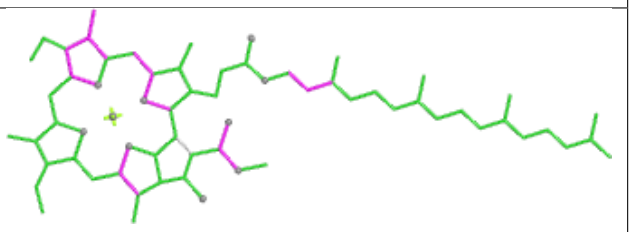


Rings

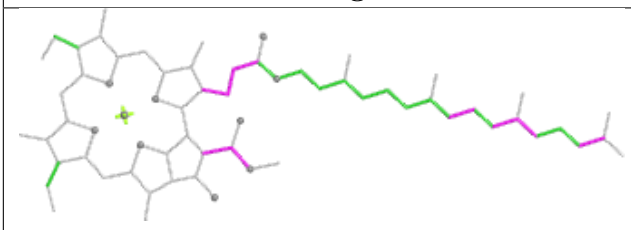
Ligand CLA C 601



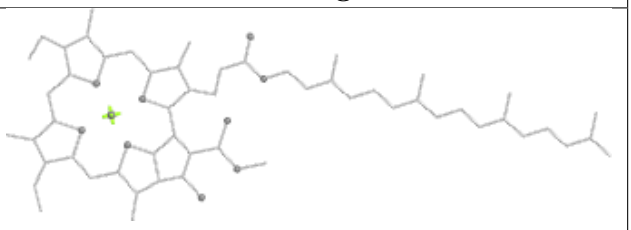
Bond lengths



Bond angles

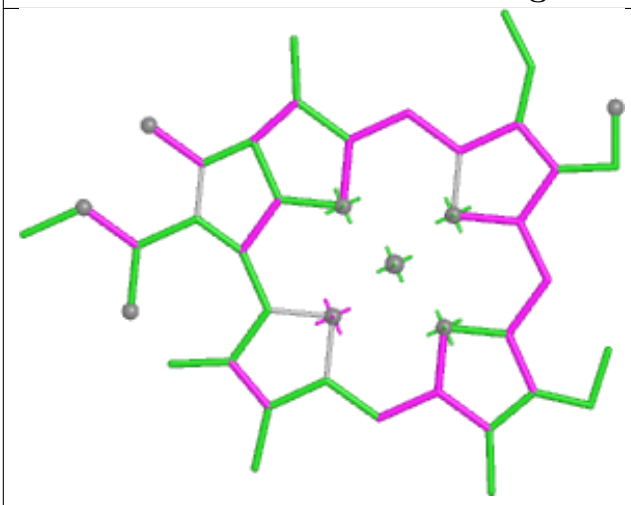


Torsions

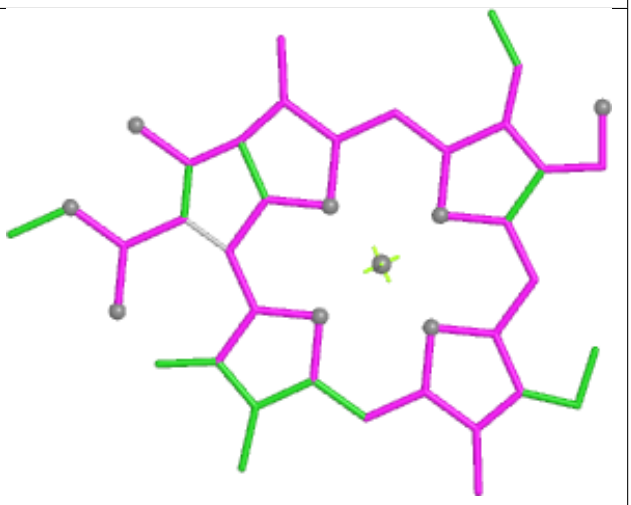


Rings

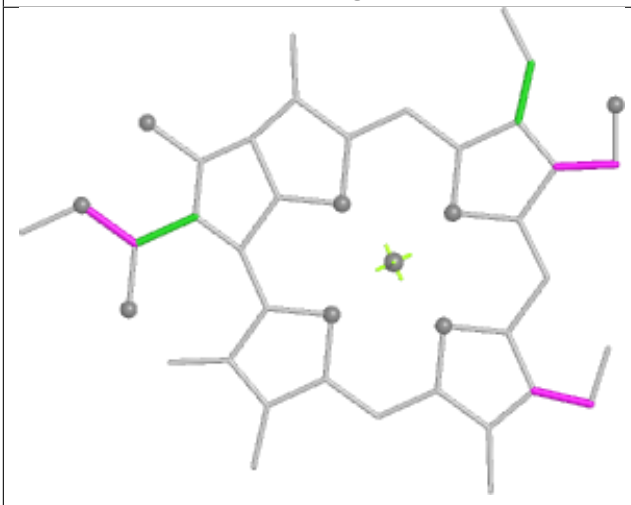
Ligand CHL r 306



Bond lengths



Bond angles

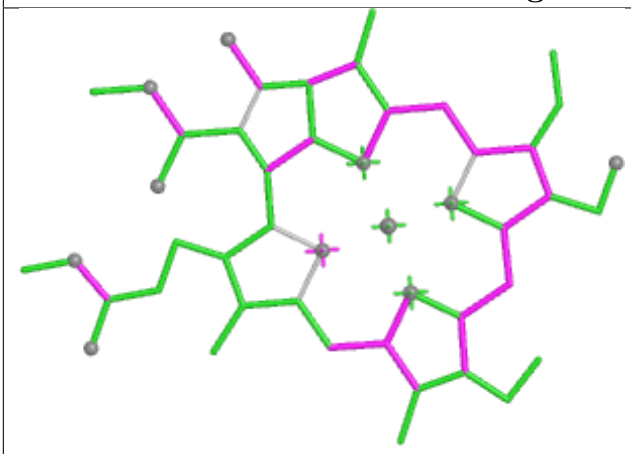


Torsions

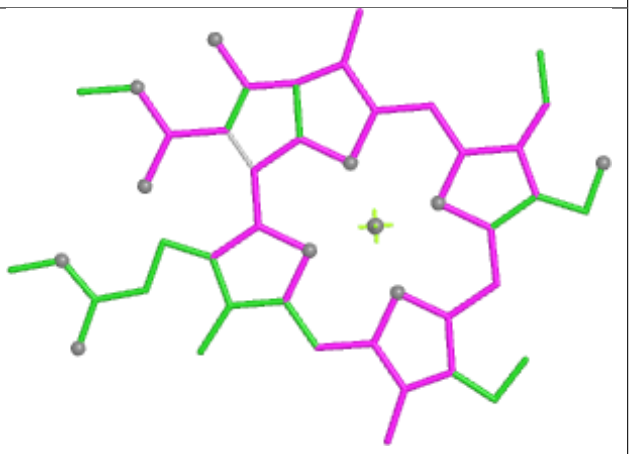


Rings

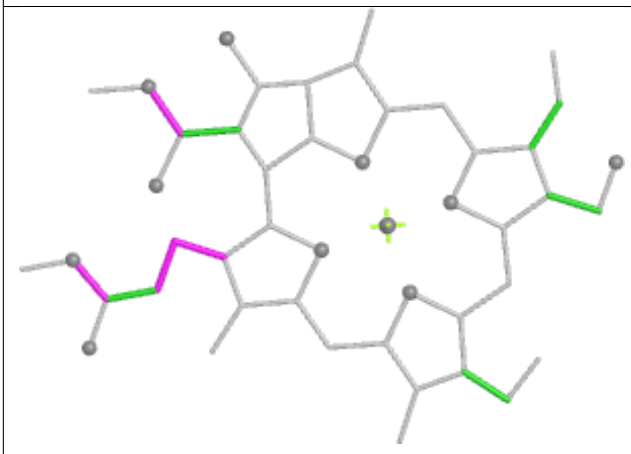
Ligand CHL u 312



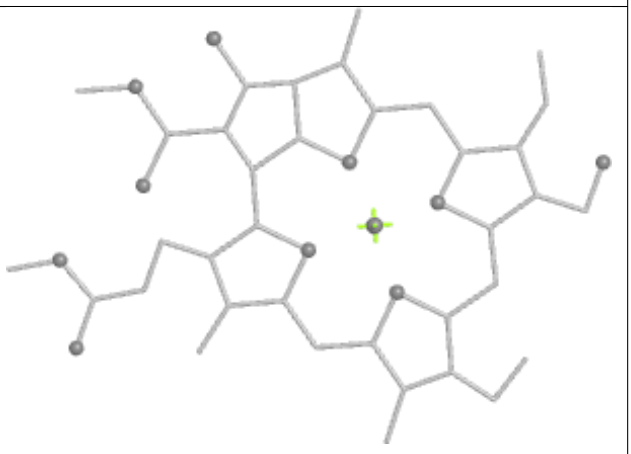
Bond lengths



Bond angles

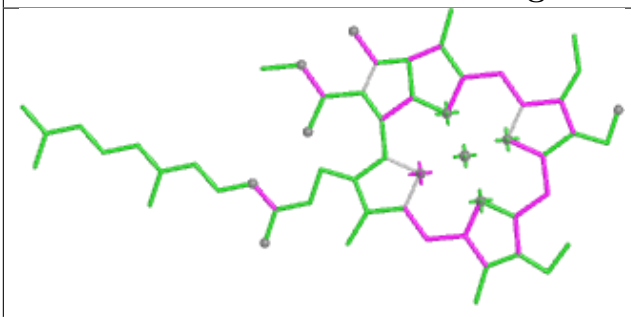


Torsions

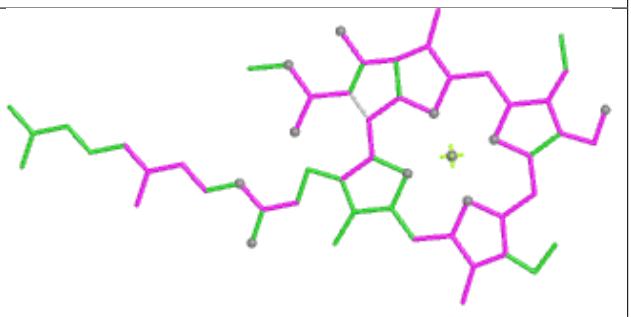


Rings

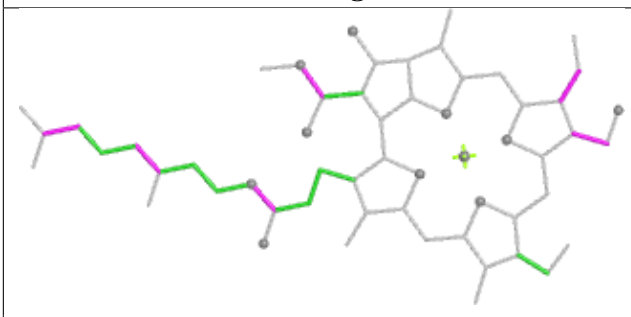
Ligand CHL 8 310



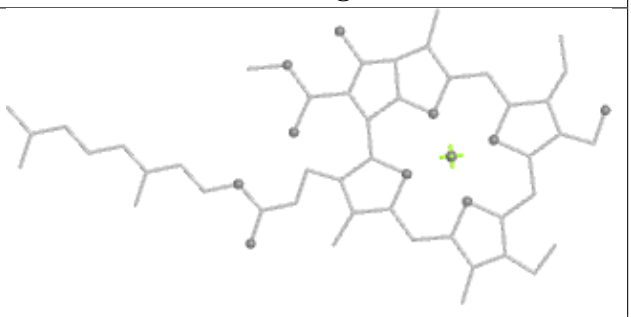
Bond lengths



Bond angles

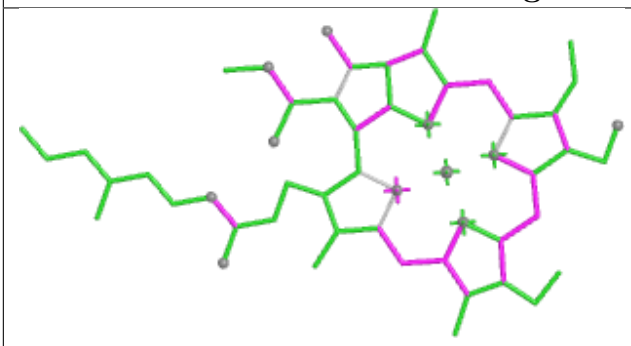


Torsions

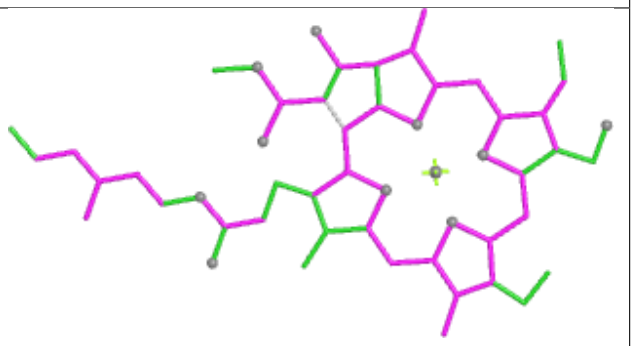


Rings

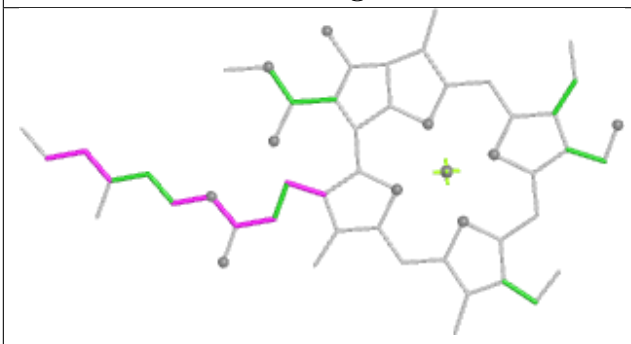
Ligand CHL Y 319



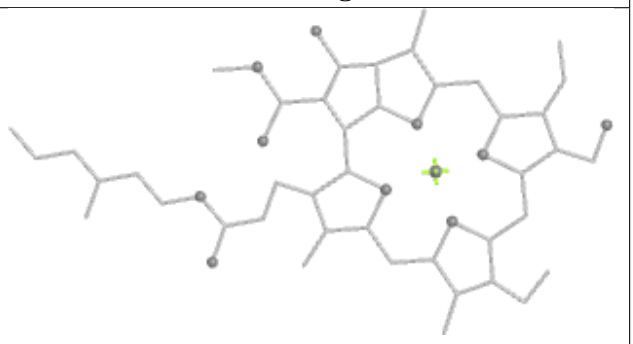
Bond lengths



Bond angles

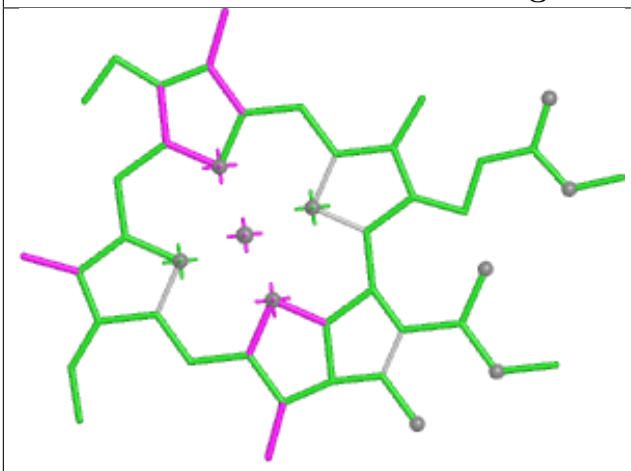


Torsions

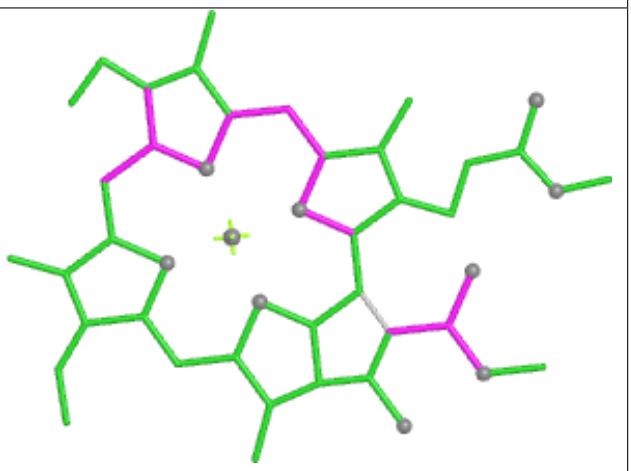


Rings

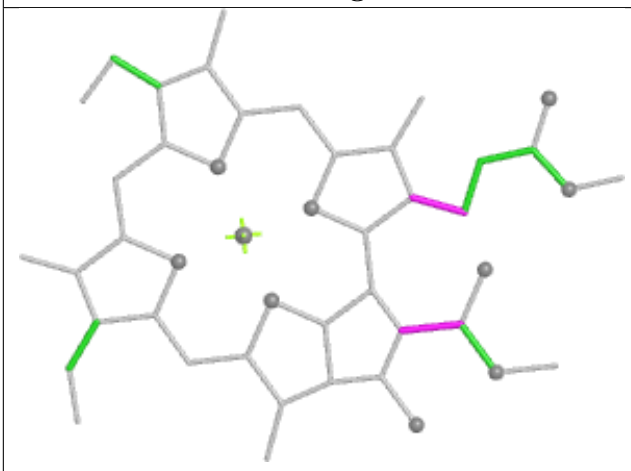
Ligand CLA c 616



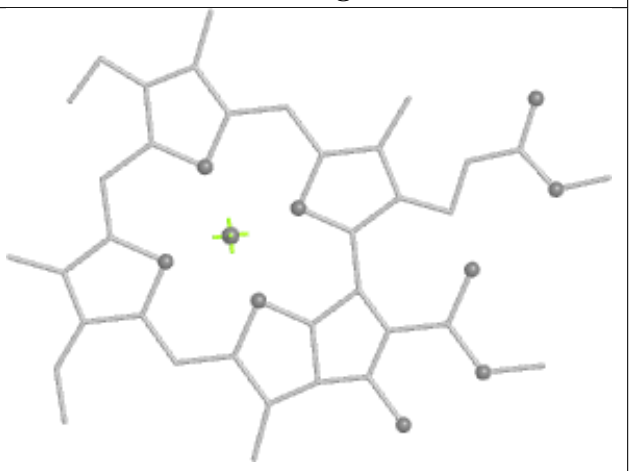
Bond lengths



Bond angles

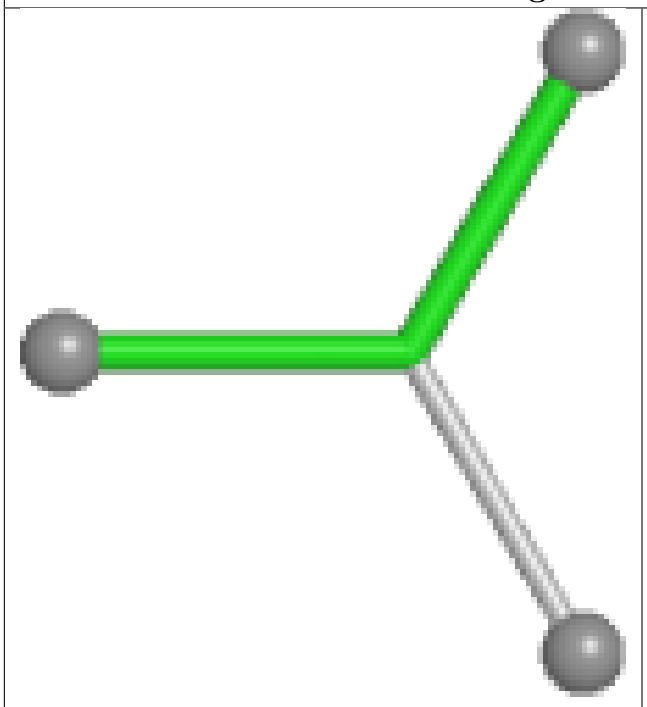


Torsions

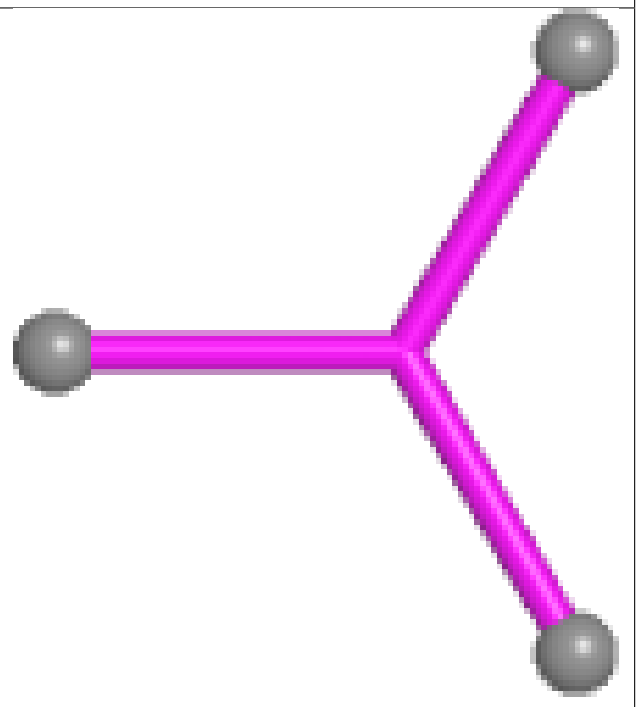


Rings

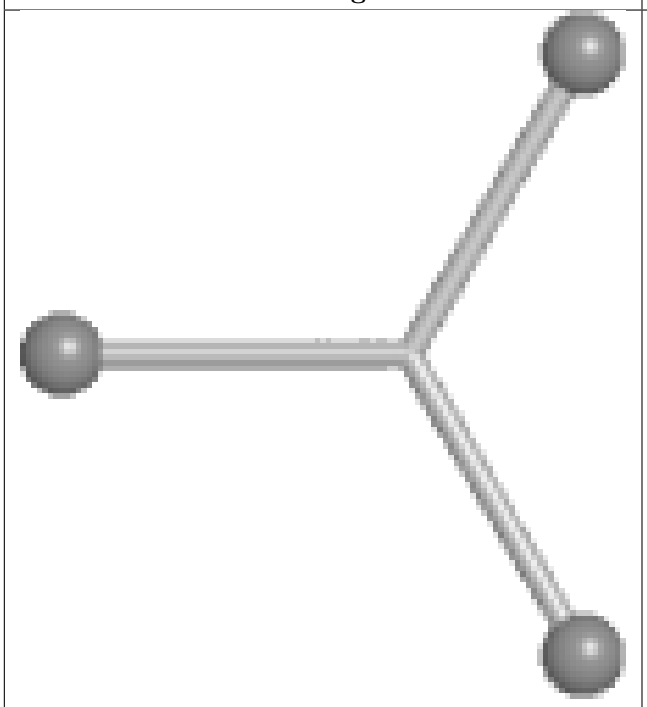
Ligand BCT a 611



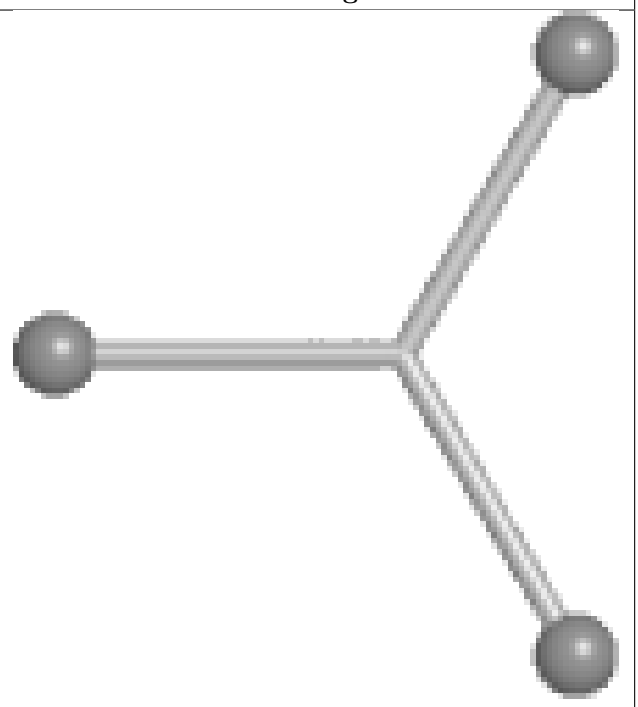
Bond lengths



Bond angles

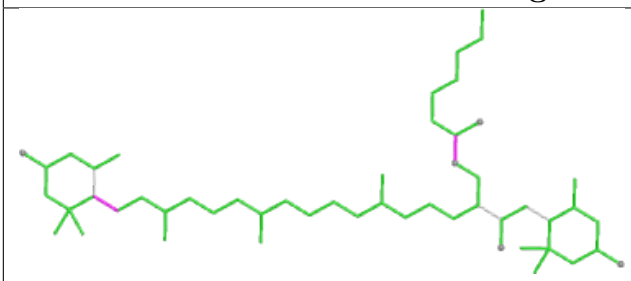


Torsions

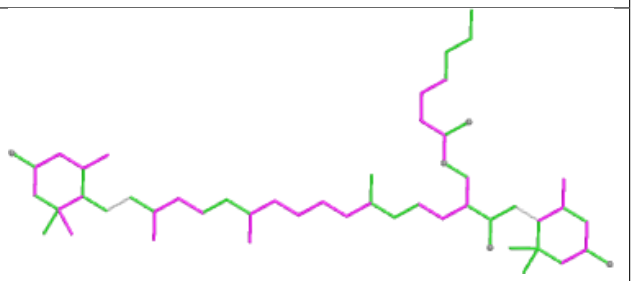


Rings

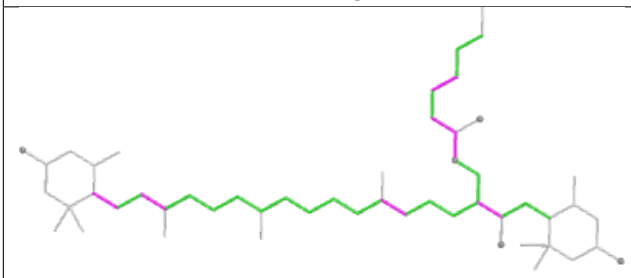
Ligand 0UR 5 301



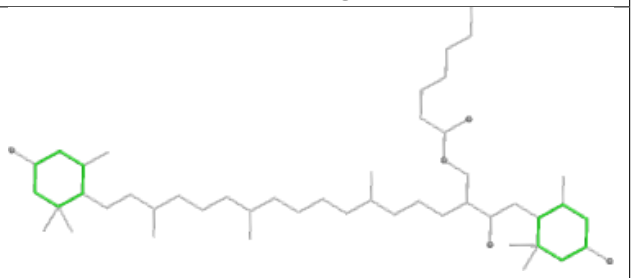
Bond lengths



Bond angles

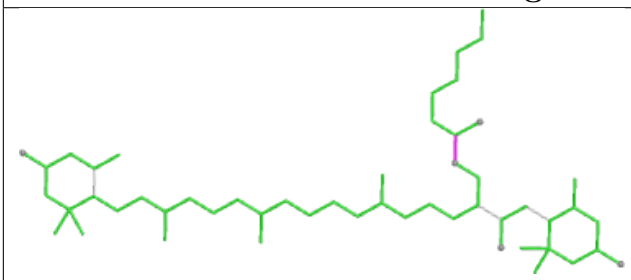


Torsions

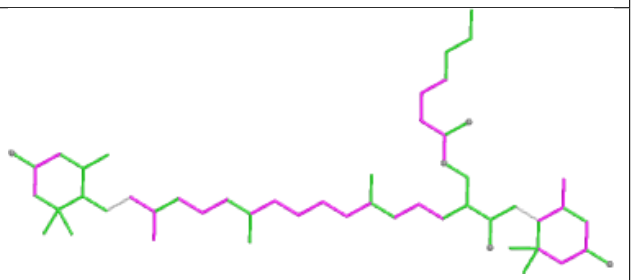


Rings

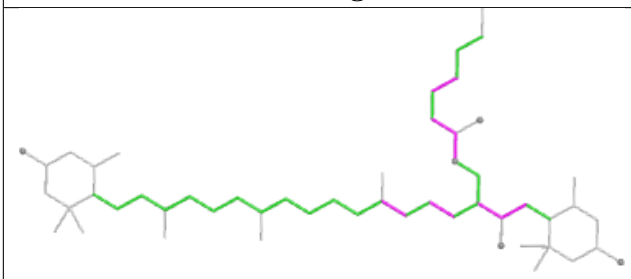
Ligand 0UR Y 301



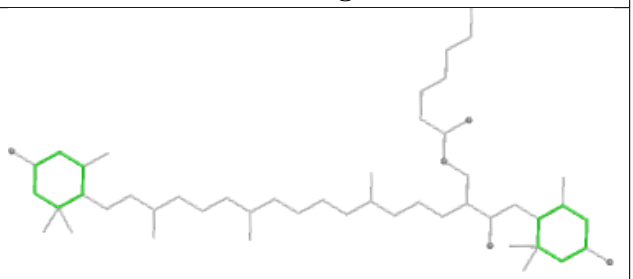
Bond lengths



Bond angles

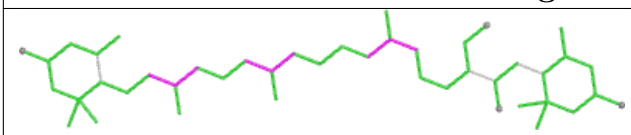


Torsions

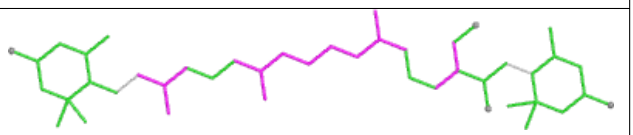


Rings

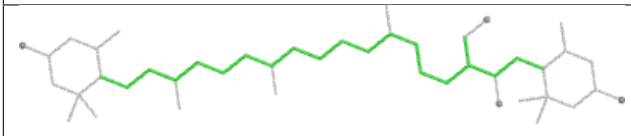
Ligand 0IE 5 303



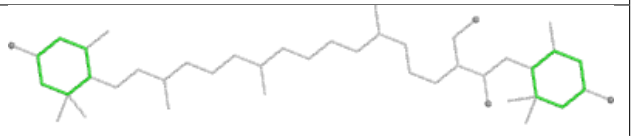
Bond lengths



Bond angles

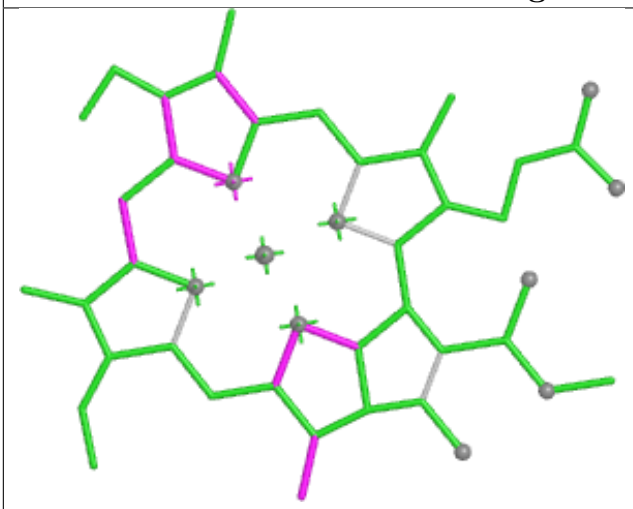


Torsions

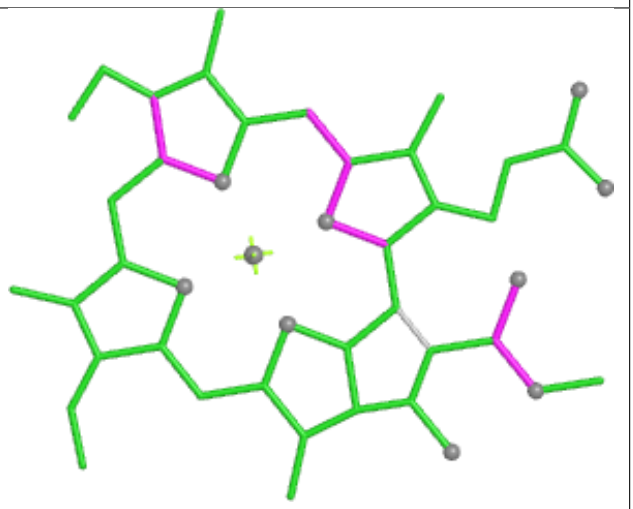


Rings

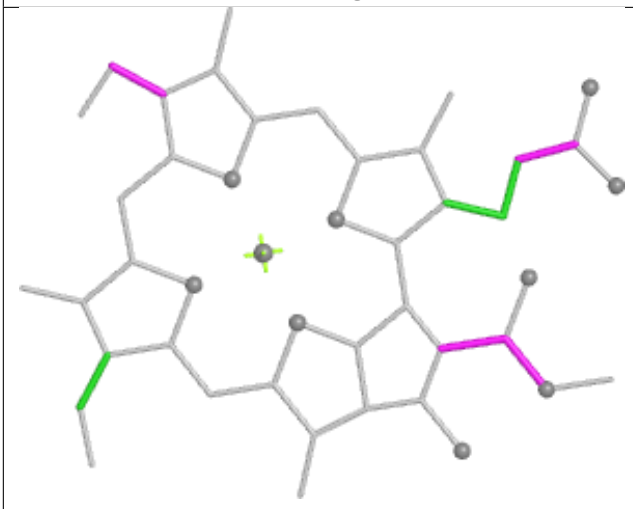
Ligand CLA 4 315



Bond lengths



Bond angles

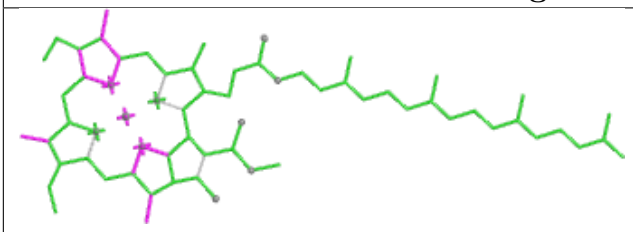


Torsions

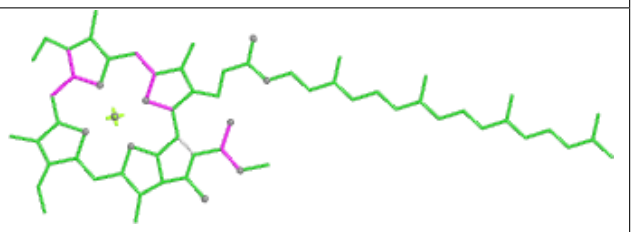


Rings

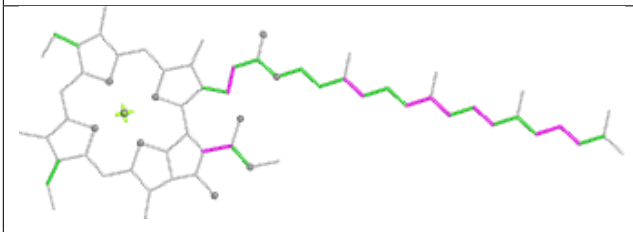
Ligand CLA c 607



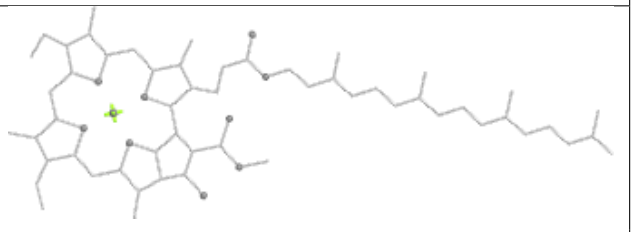
Bond lengths



Bond angles

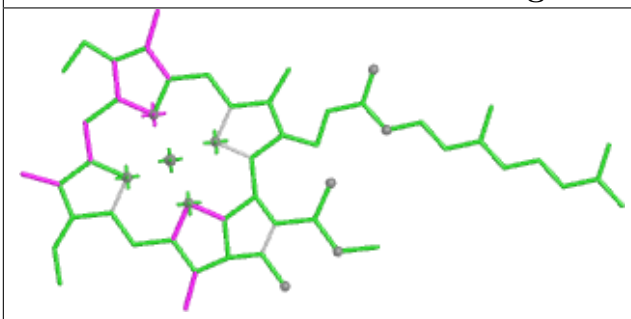


Torsions

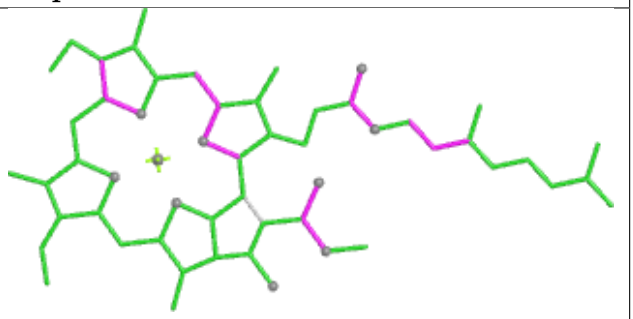


Rings

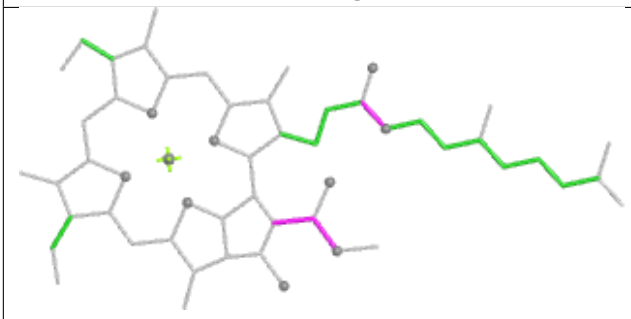
Ligand CLA p 314



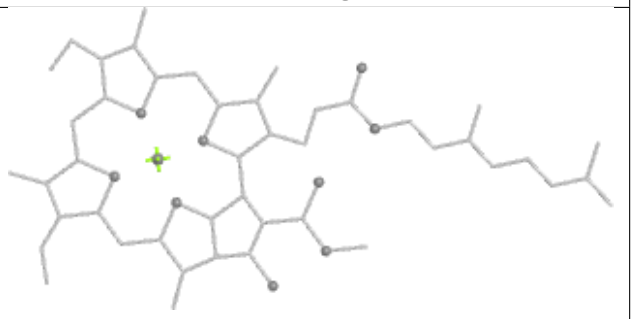
Bond lengths



Bond angles

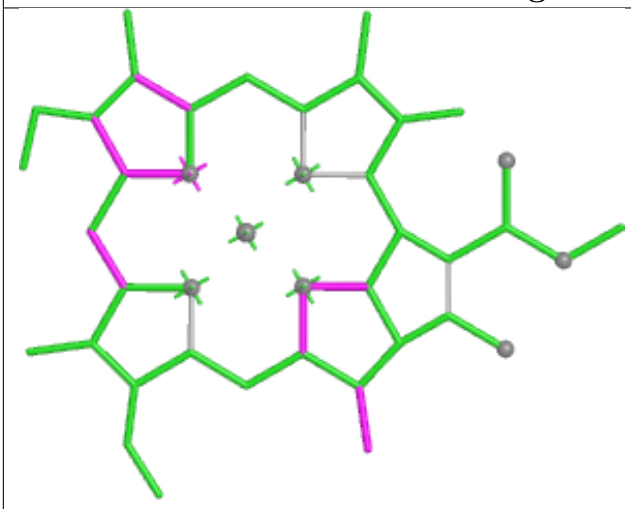


Torsions

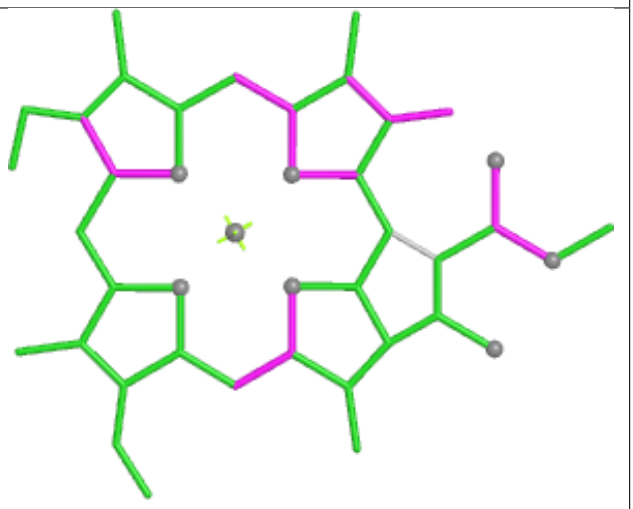


Rings

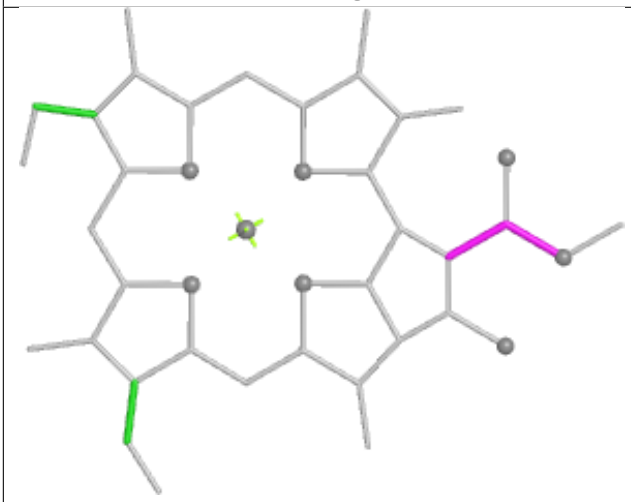
Ligand CLA a 610



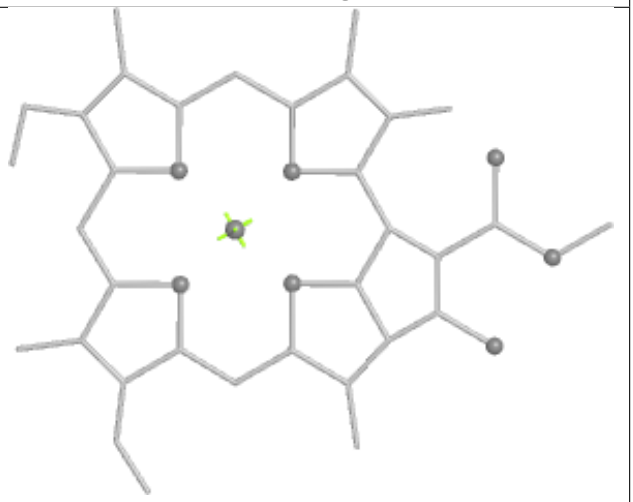
Bond lengths



Bond angles

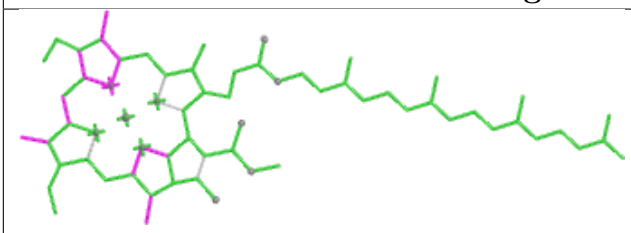


Torsions

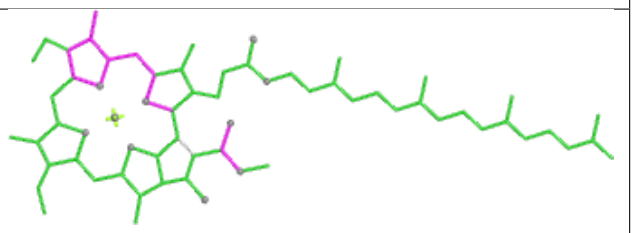


Rings

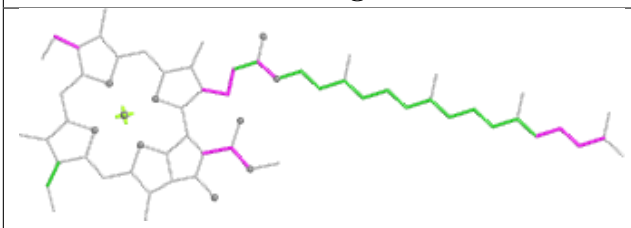
Ligand CLA A 603



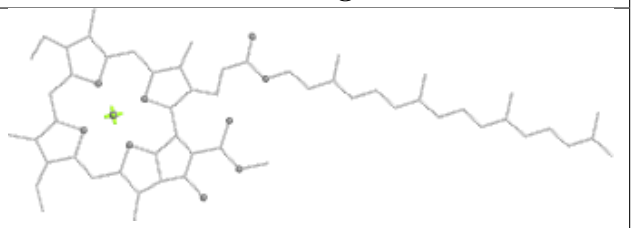
Bond lengths



Bond angles

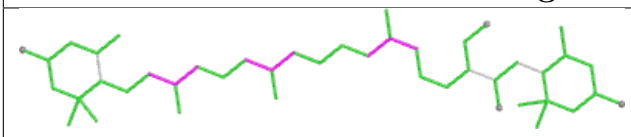


Torsions

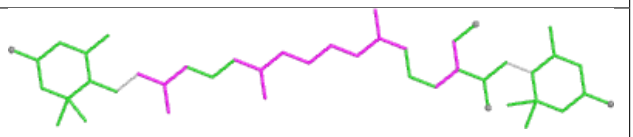


Rings

Ligand 0IE 7 303



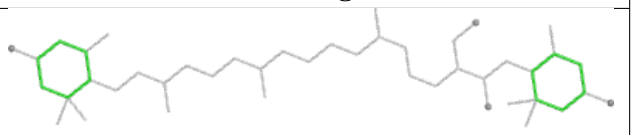
Bond lengths



Bond angles

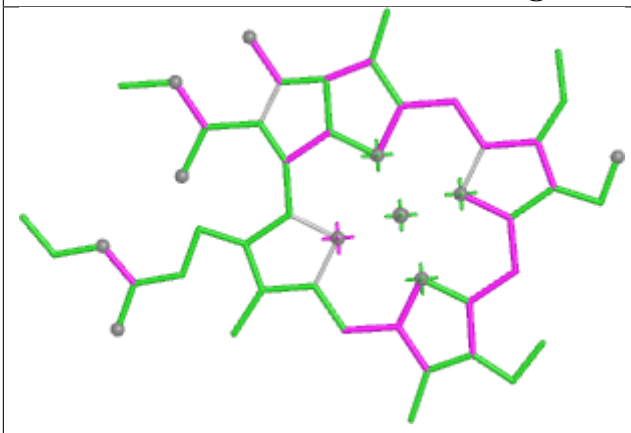


Torsions

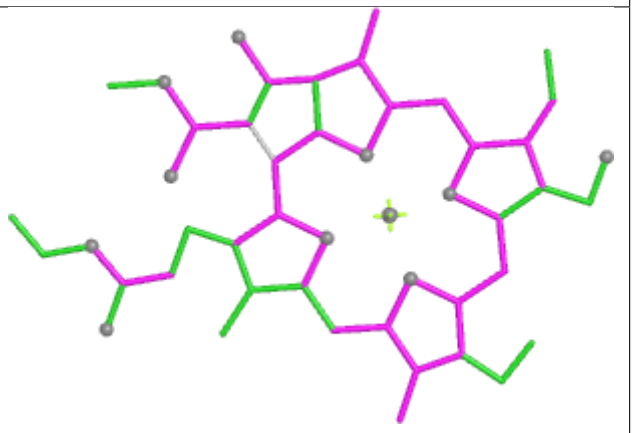


Rings

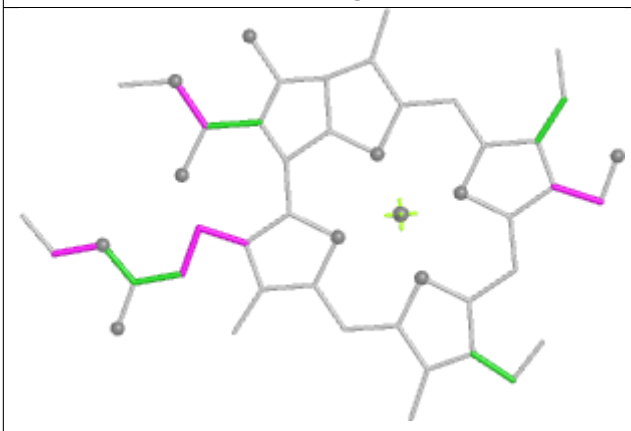
Ligand CHL 6 304



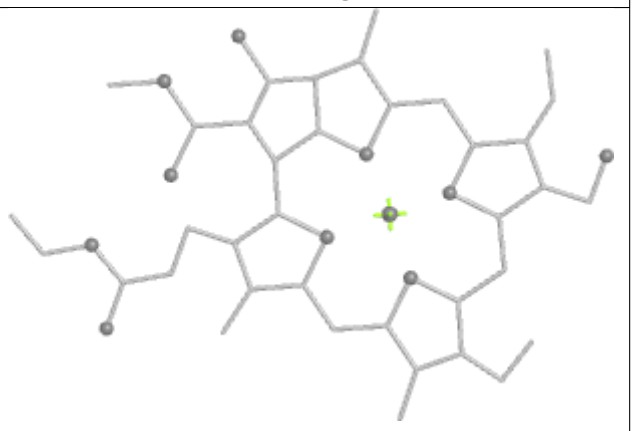
Bond lengths



Bond angles

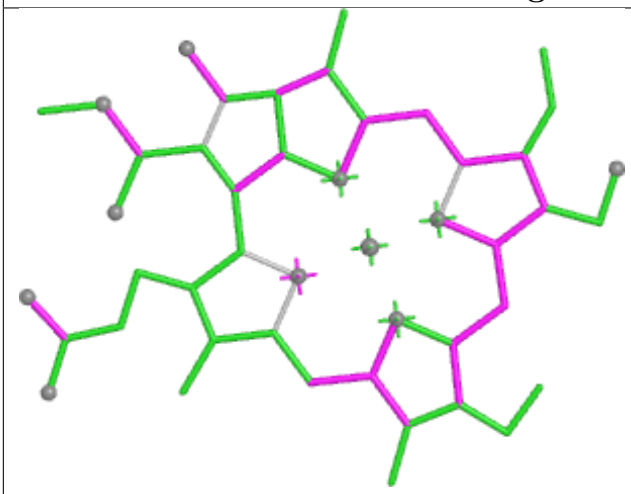


Torsions

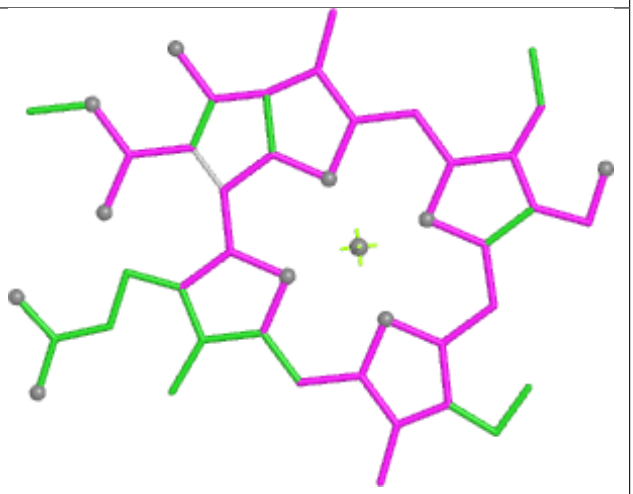


Rings

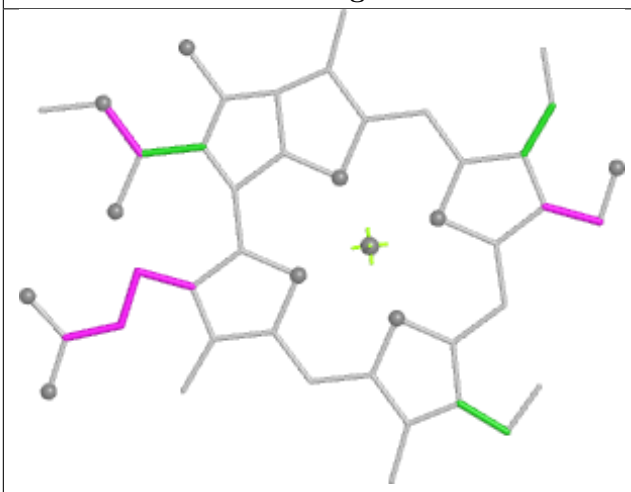
Ligand CHL 9 309



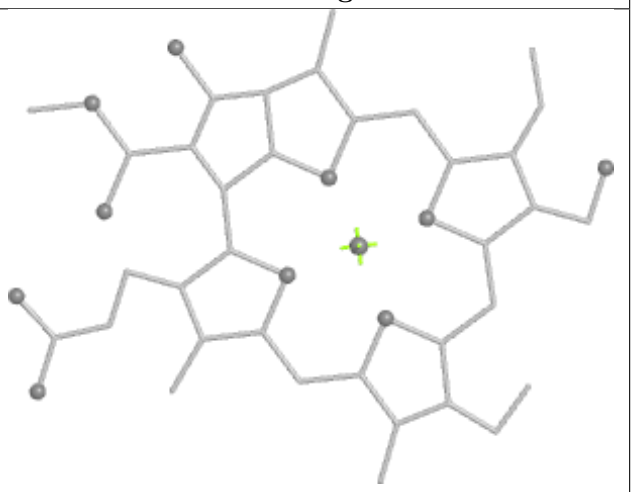
Bond lengths



Bond angles

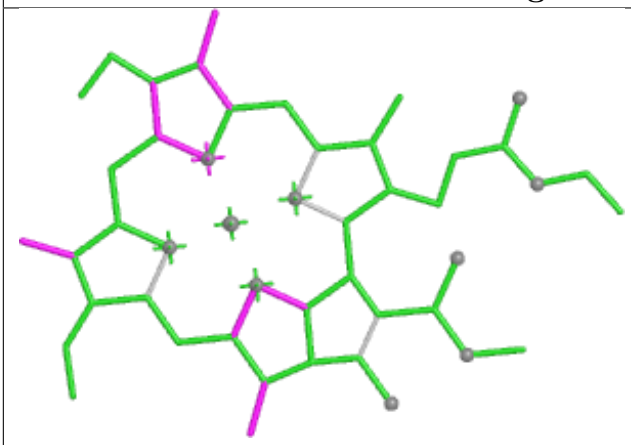


Torsions

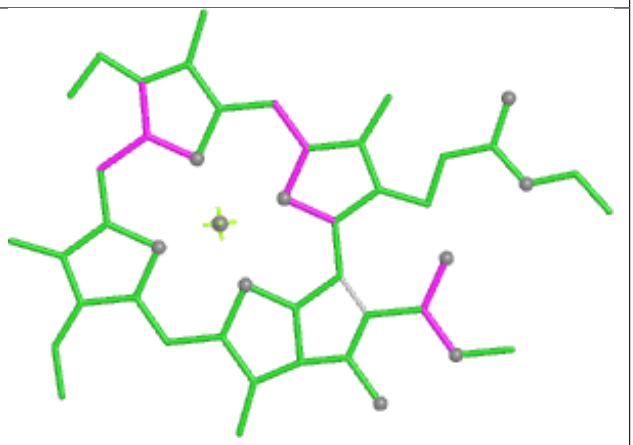


Rings

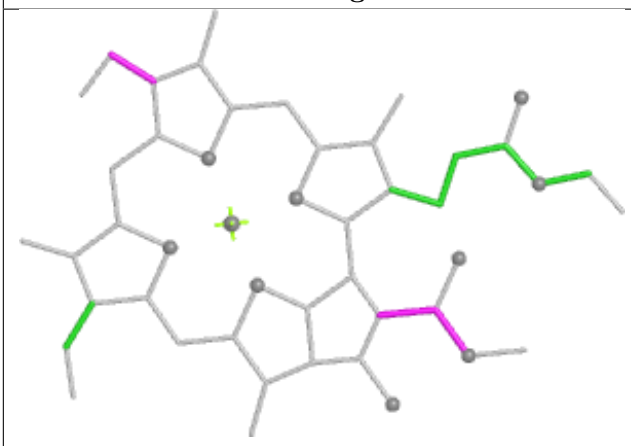
Ligand CLA b 616



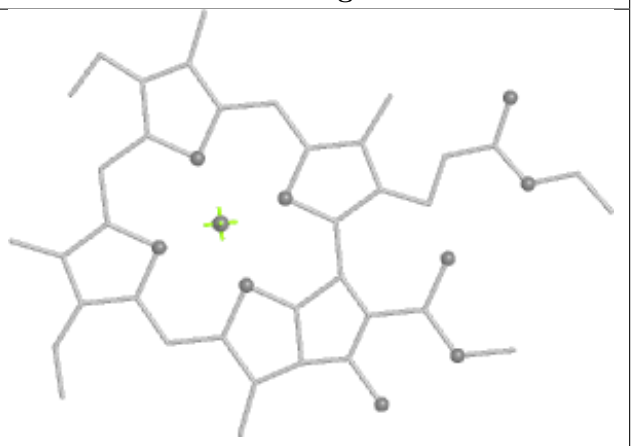
Bond lengths



Bond angles

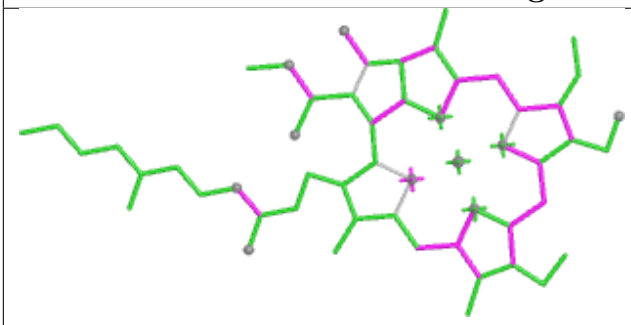


Torsions

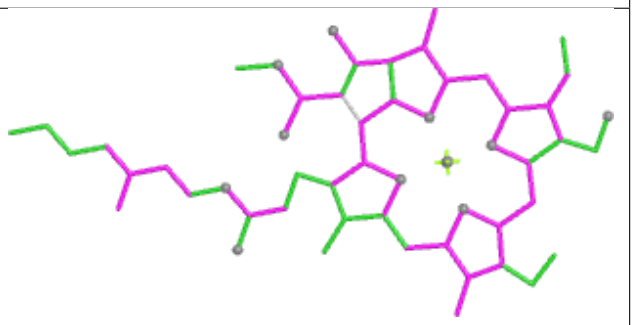


Rings

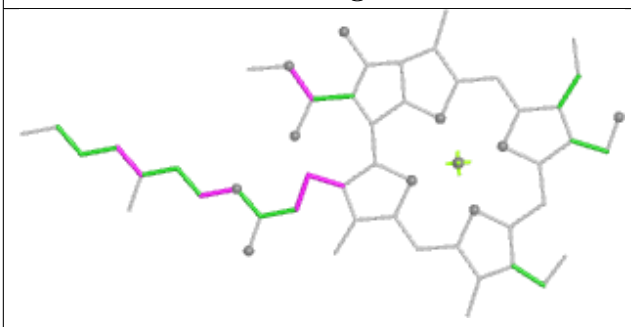
Ligand CHL 8 303



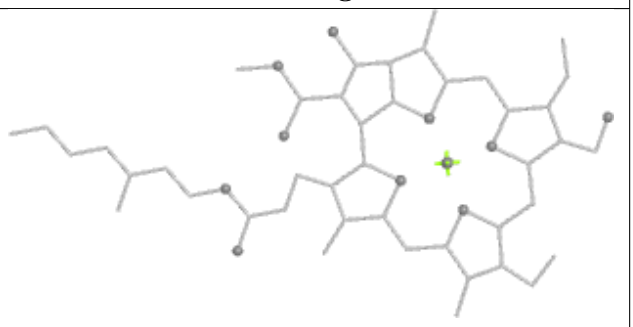
Bond lengths



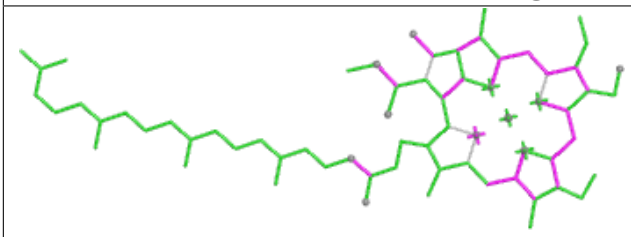
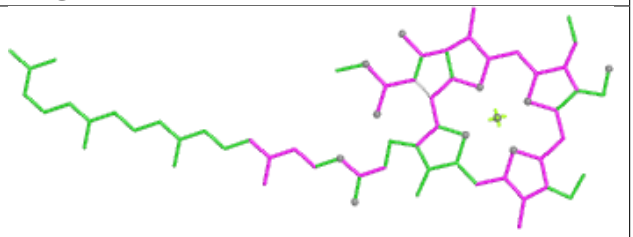
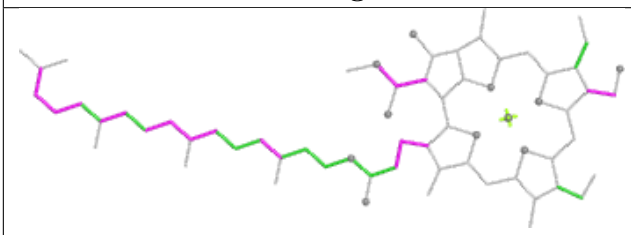
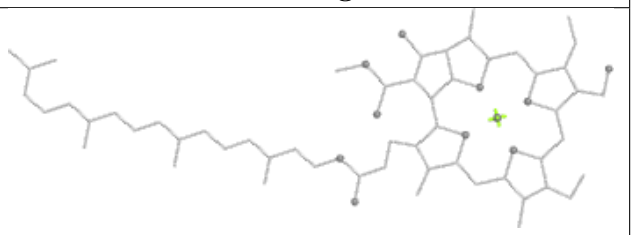
Bond angles

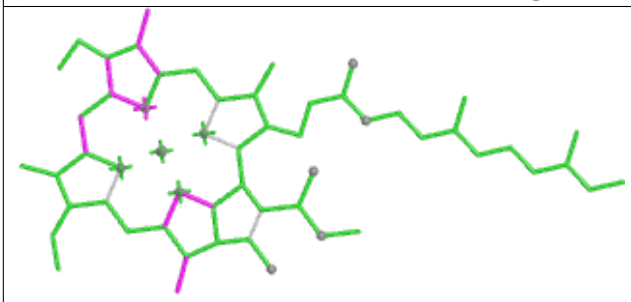
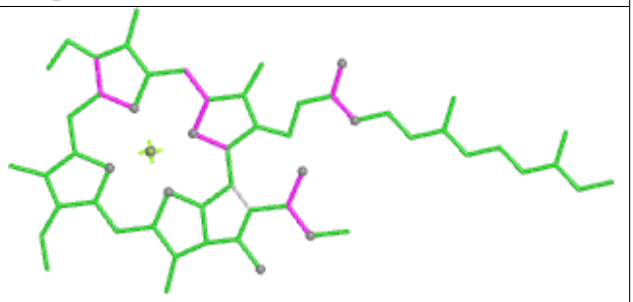
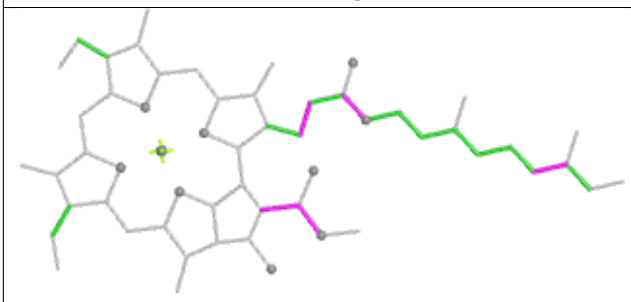
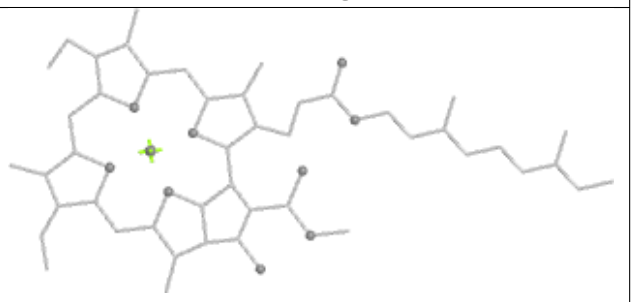


Torsions

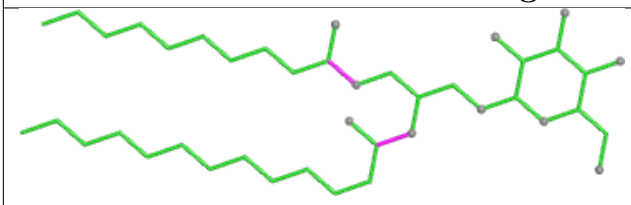


Rings

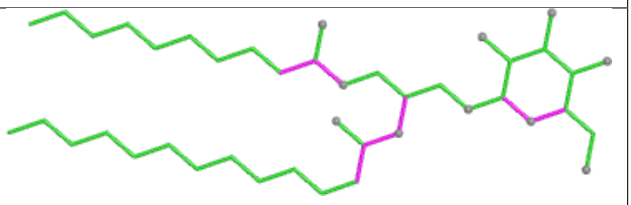
Ligand CHL g 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

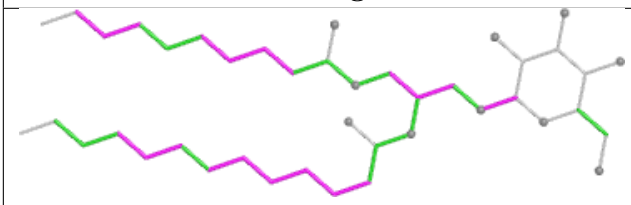
Ligand LMG C 618



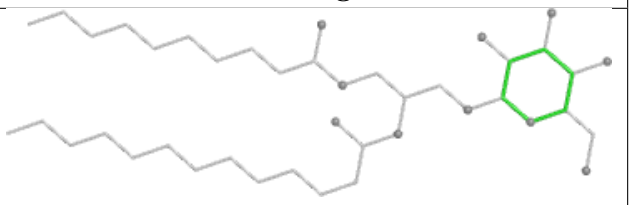
Bond lengths



Bond angles

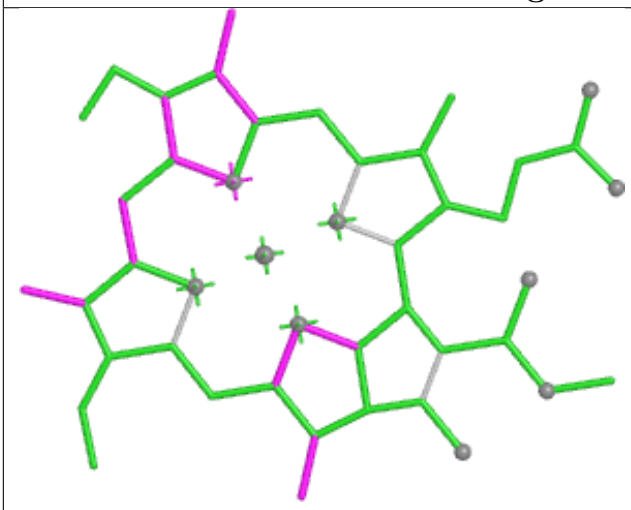


Torsions

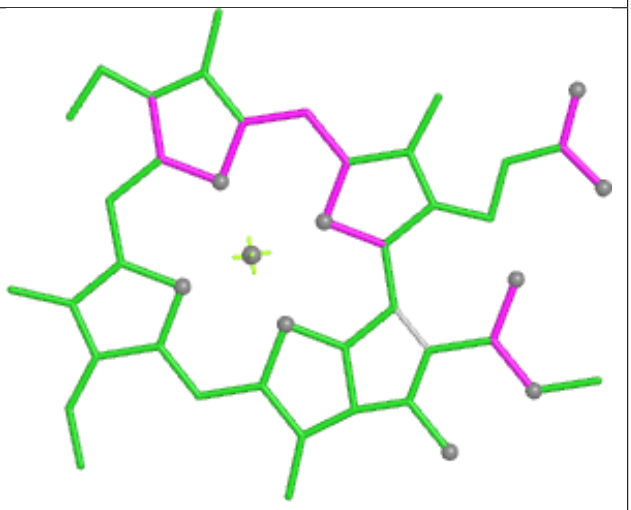


Rings

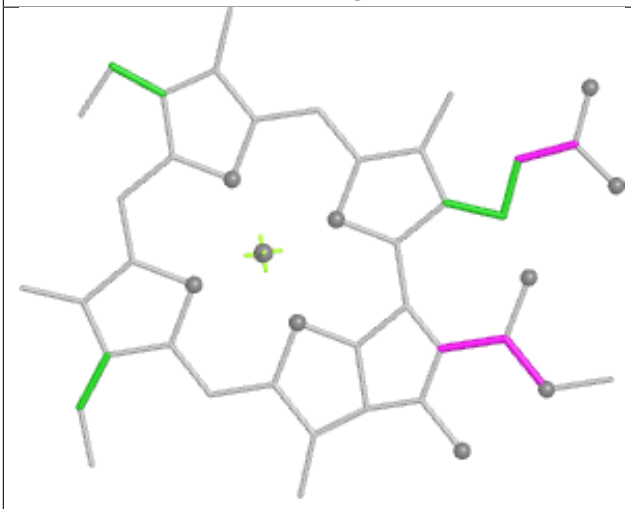
Ligand CLA S 611



Bond lengths



Bond angles

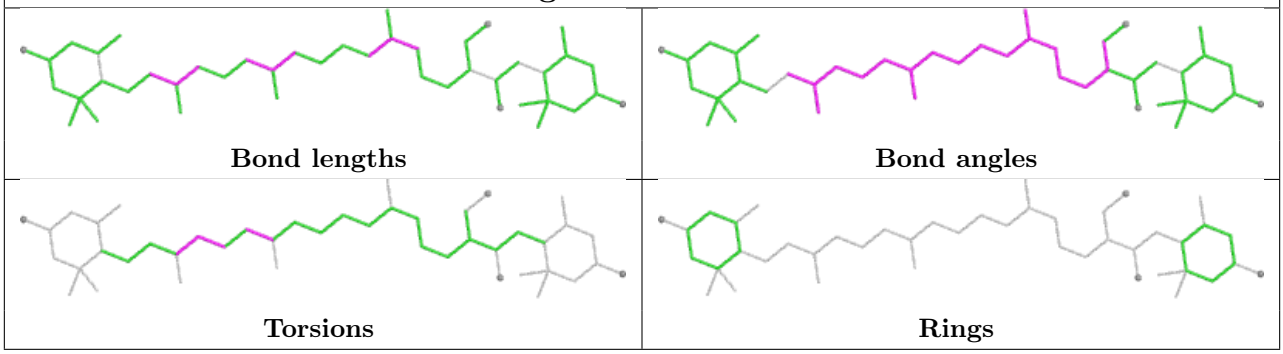


Torsions

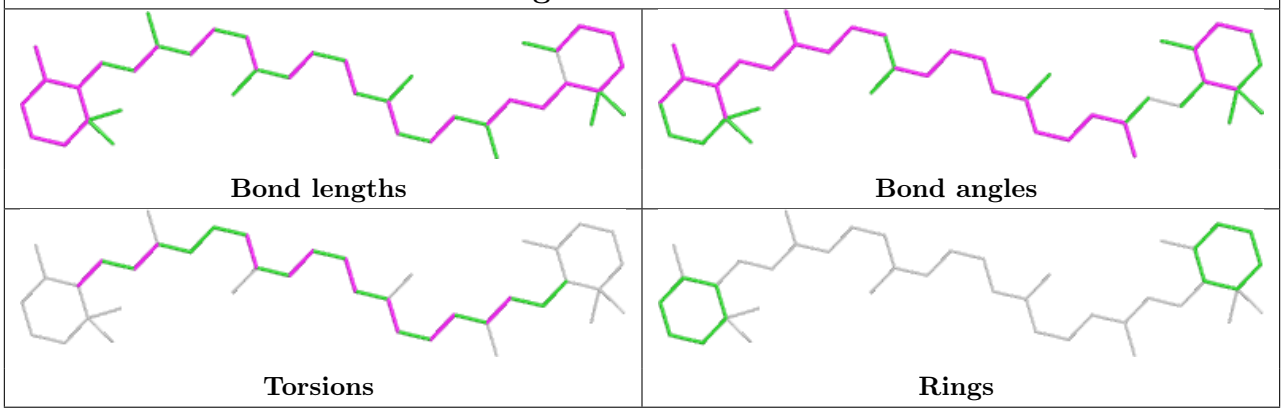


Rings

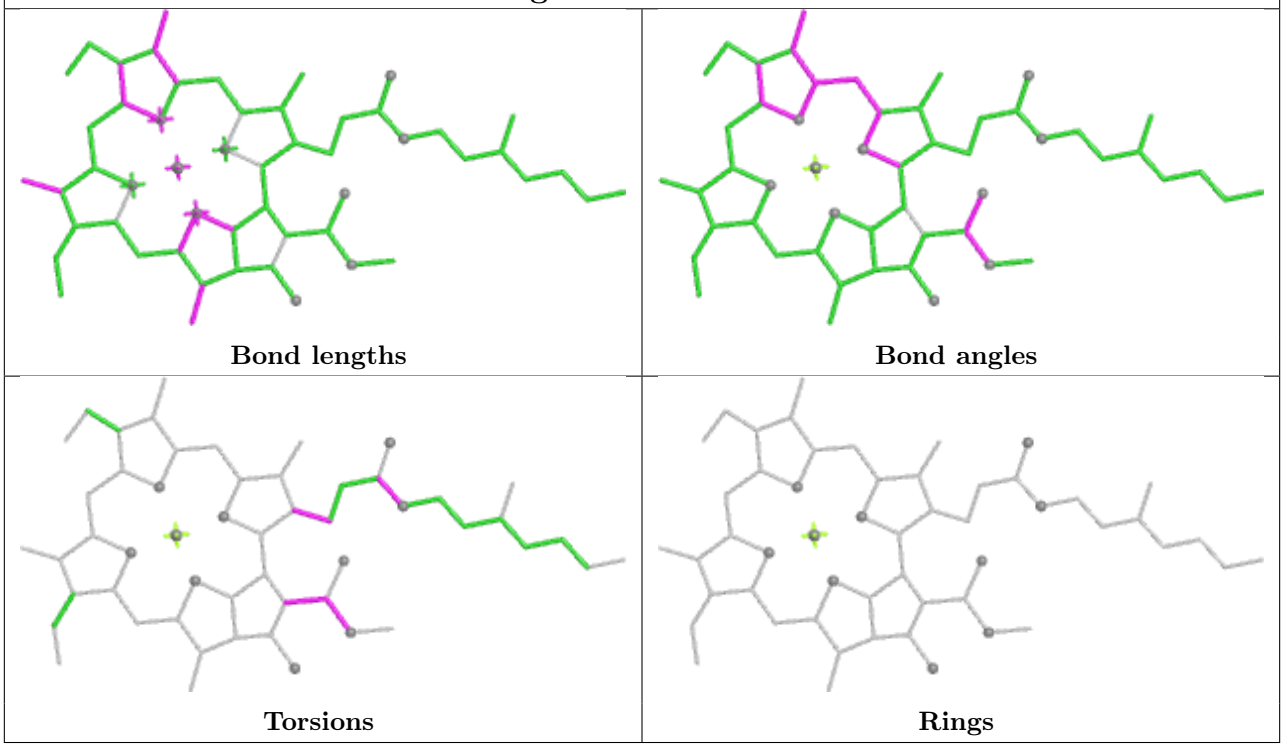
Ligand 0IE 9 303

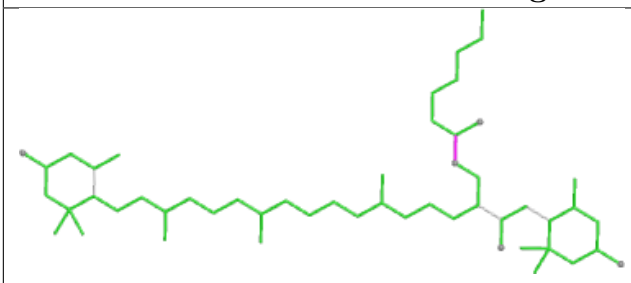
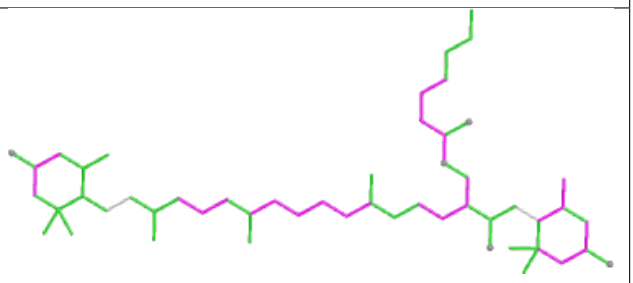
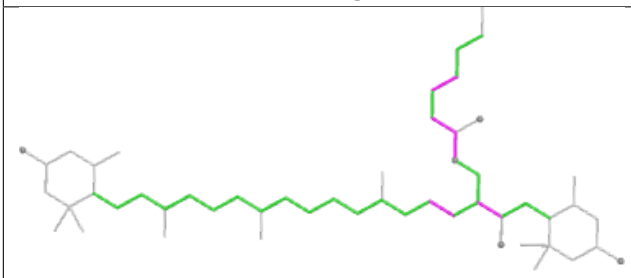
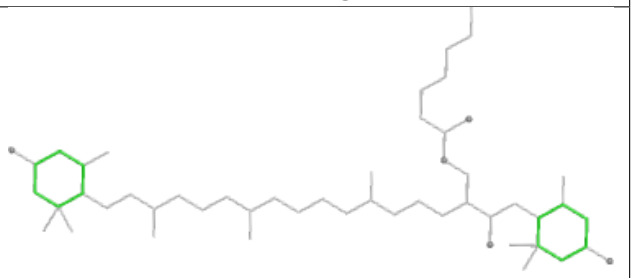


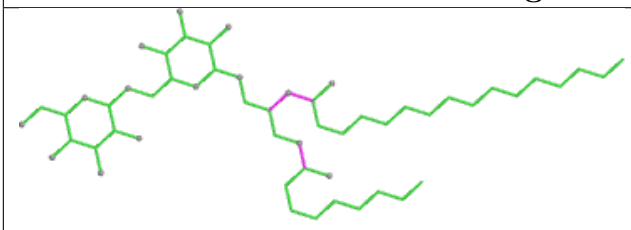
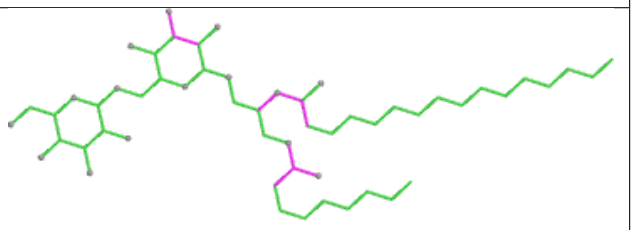
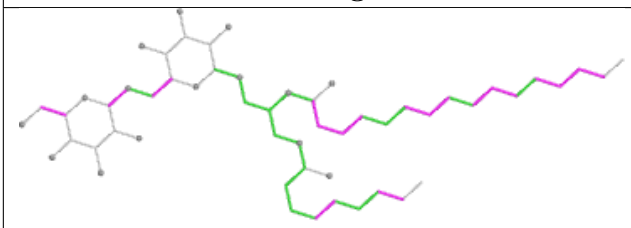
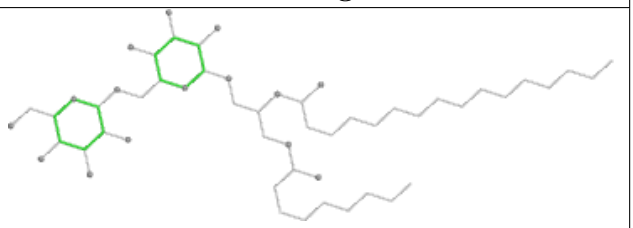
Ligand 8CT c 615



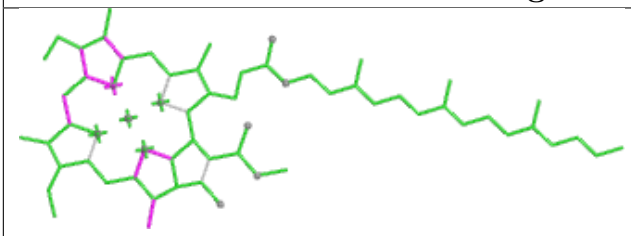
Ligand CLA c 606



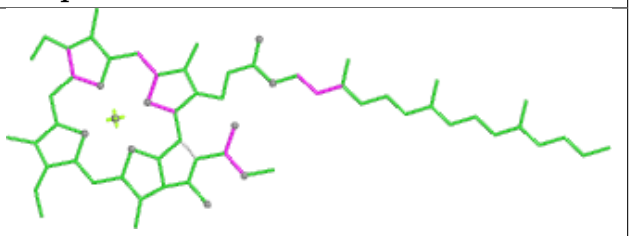
Ligand 0UR 7 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD c 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

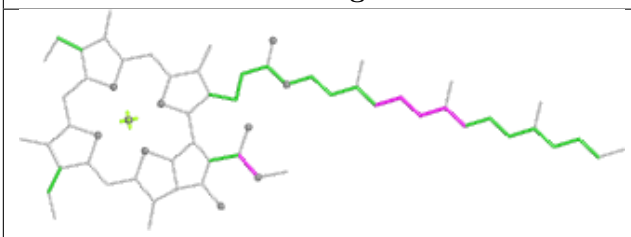
Ligand CLA q 313



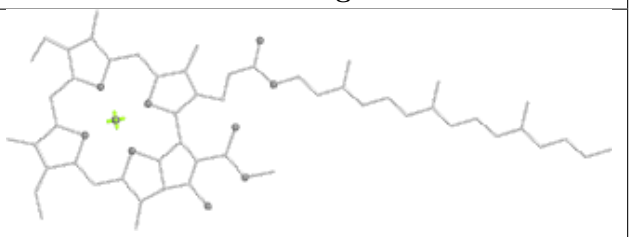
Bond lengths



Bond angles

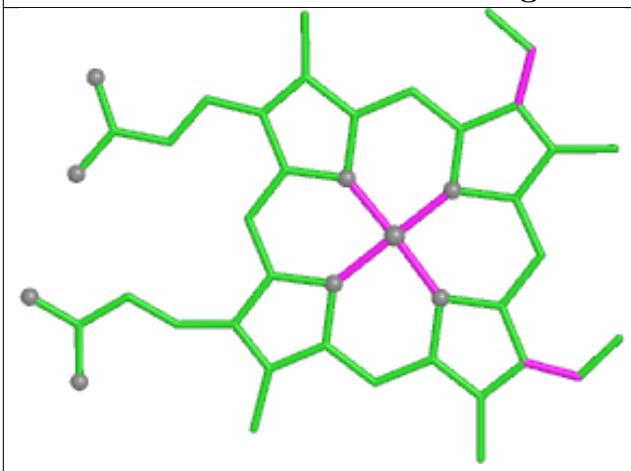


Torsions

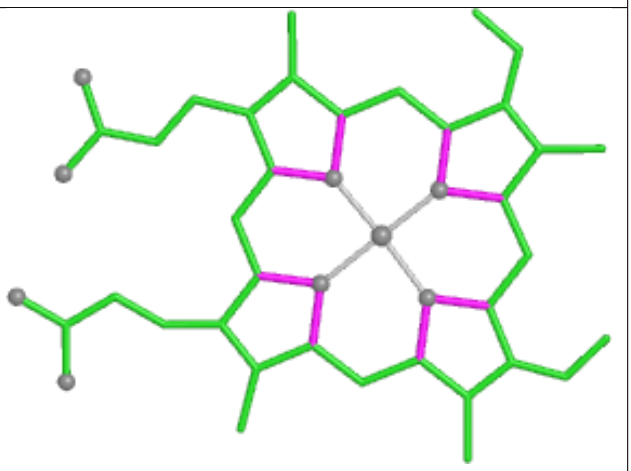


Rings

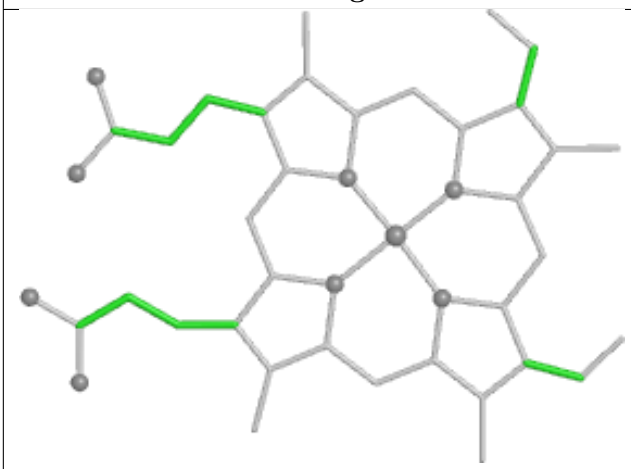
Ligand HEM E 201



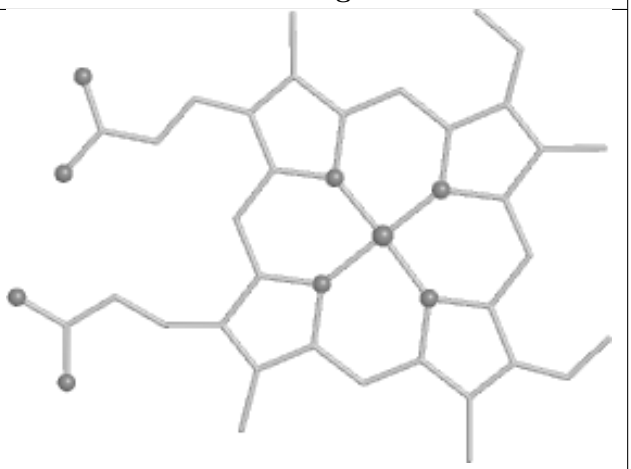
Bond lengths



Bond angles

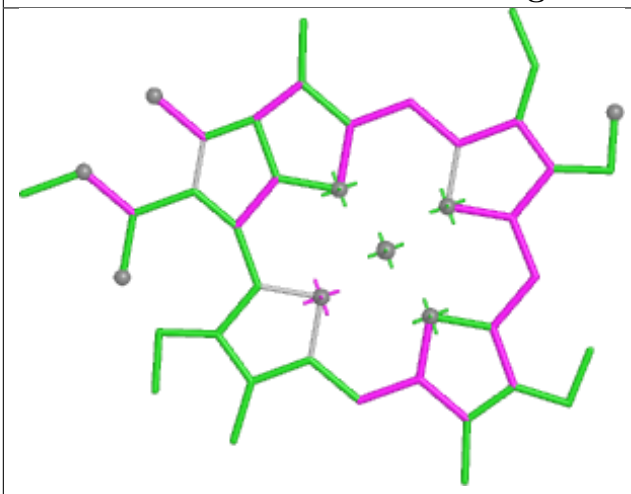


Torsions

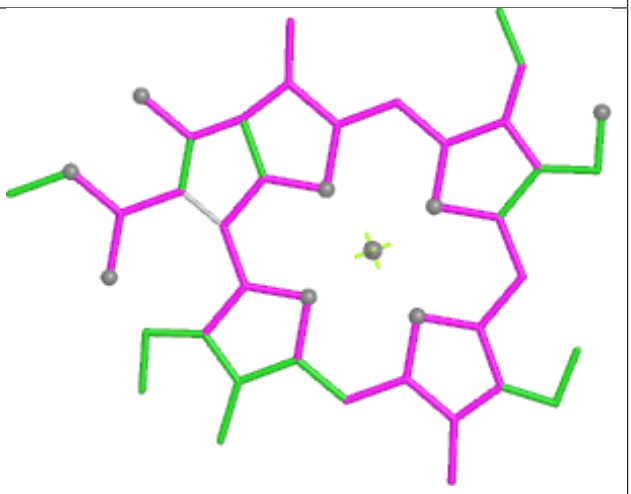


Rings

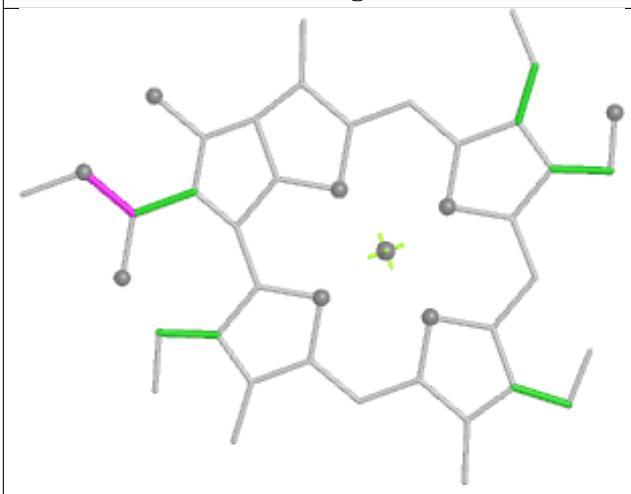
Ligand CHL 6 308



Bond lengths



Bond angles

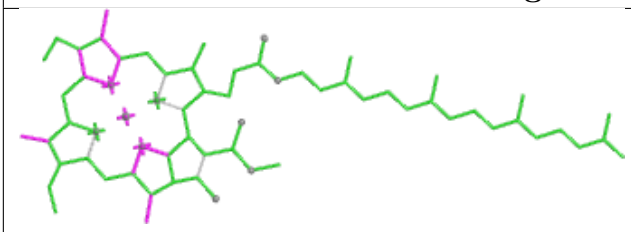


Torsions

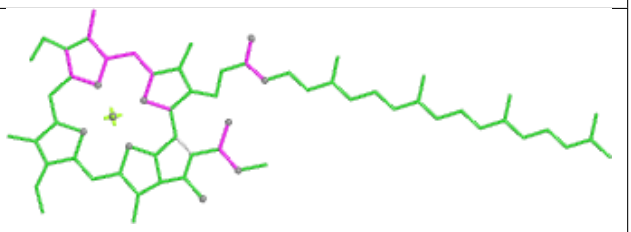


Rings

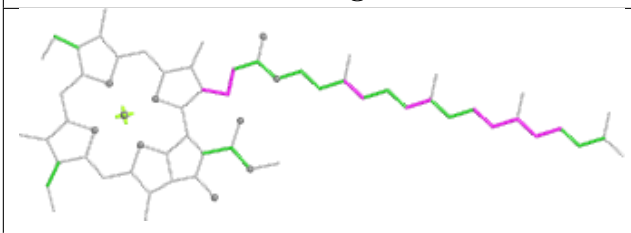
Ligand CLA B 603



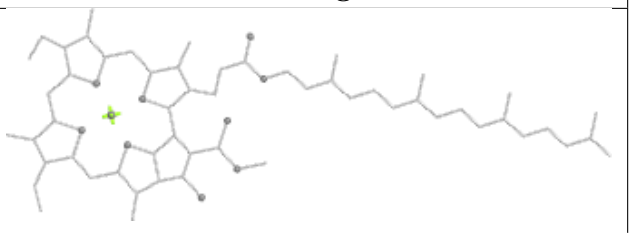
Bond lengths



Bond angles

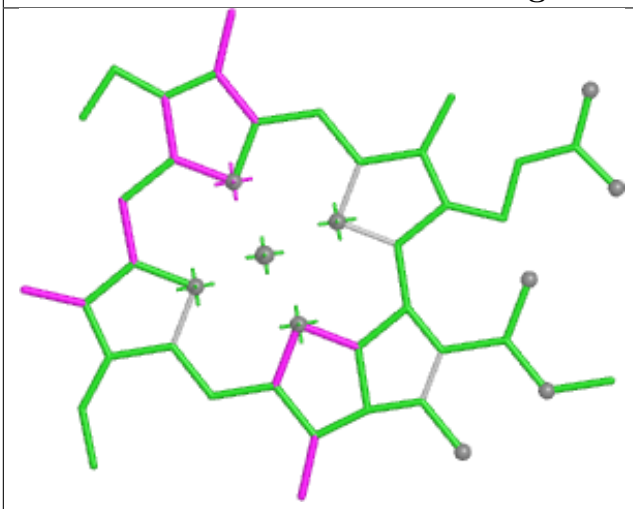


Torsions

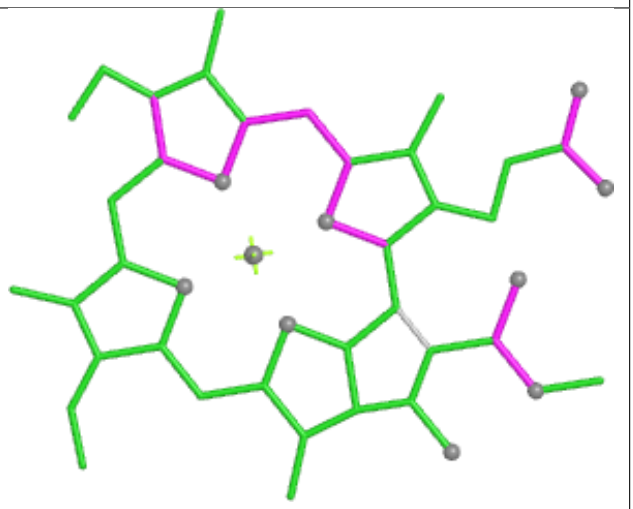


Rings

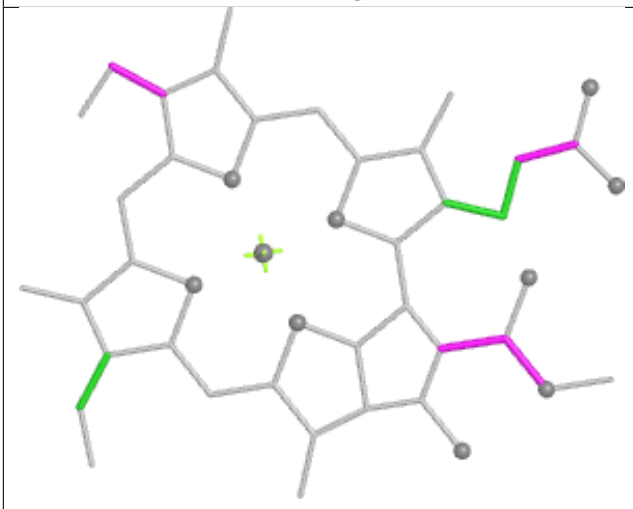
Ligand CLA 6 315



Bond lengths



Bond angles

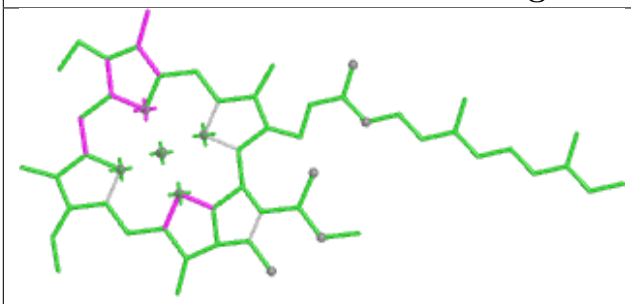


Torsions

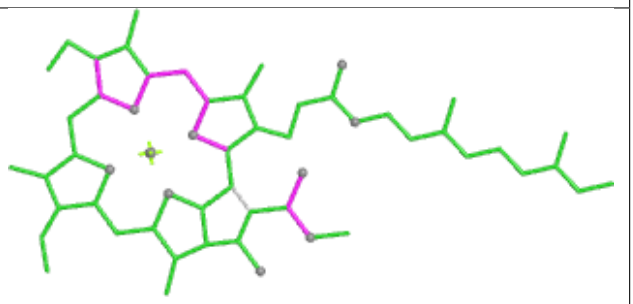


Rings

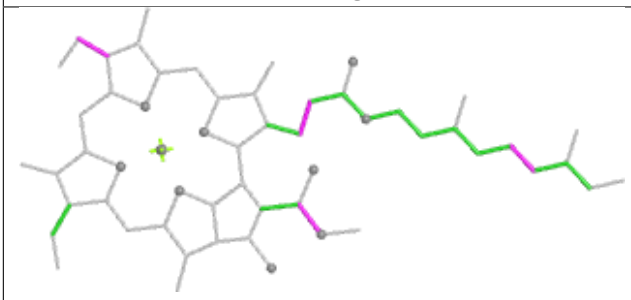
Ligand CLA 9 306



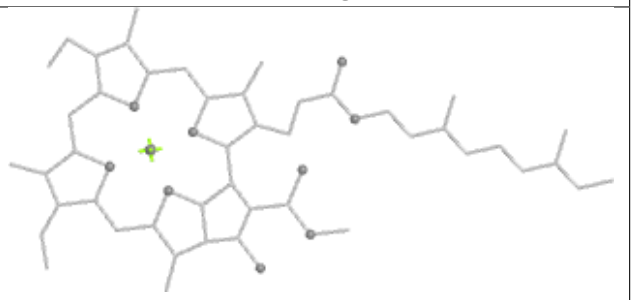
Bond lengths



Bond angles

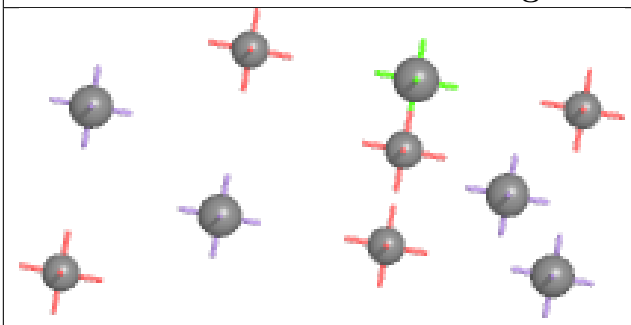


Torsions

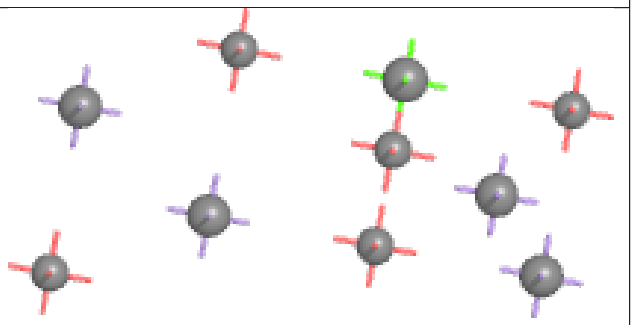


Rings

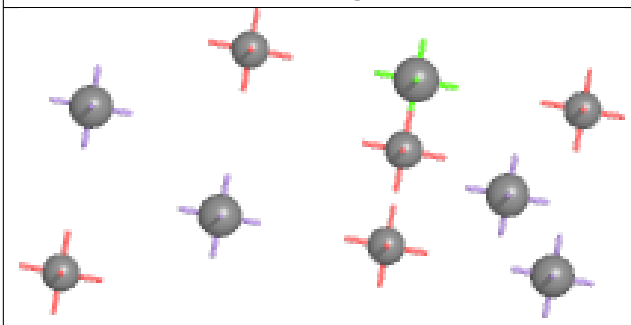
Ligand OEX A 602



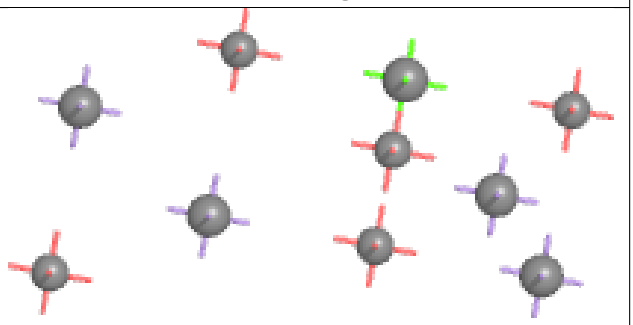
Bond lengths



Bond angles

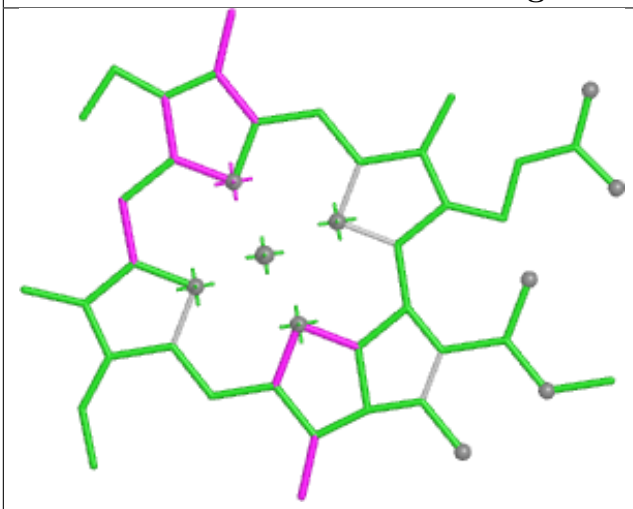


Torsions

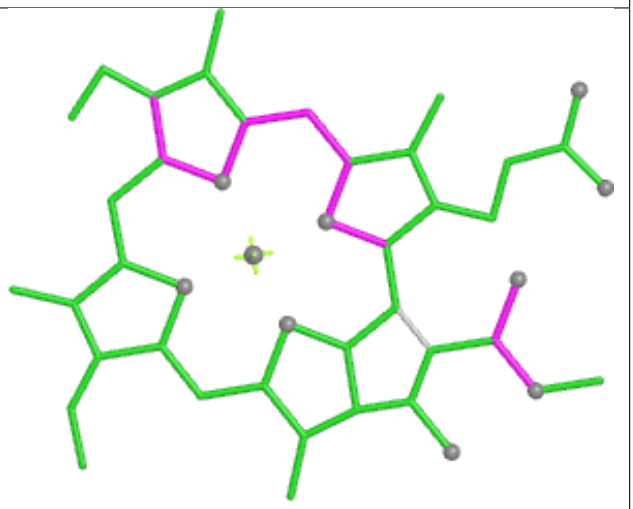


Rings

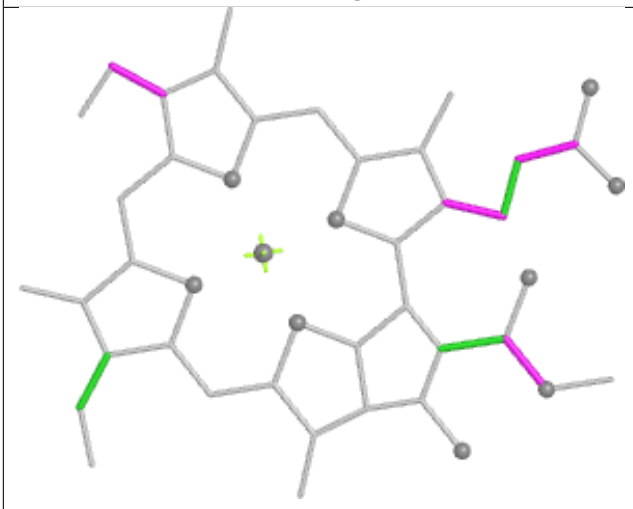
Ligand CLA S 616



Bond lengths



Bond angles

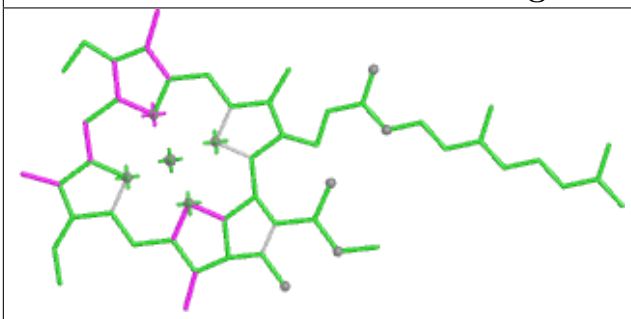


Torsions

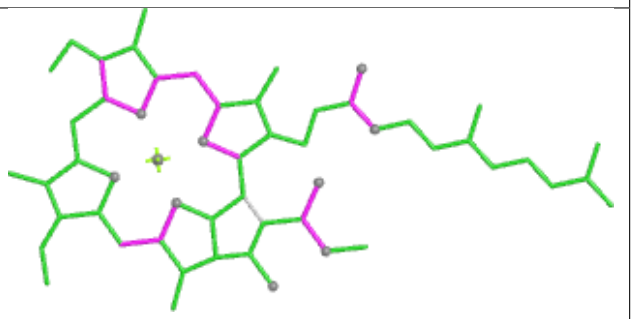


Rings

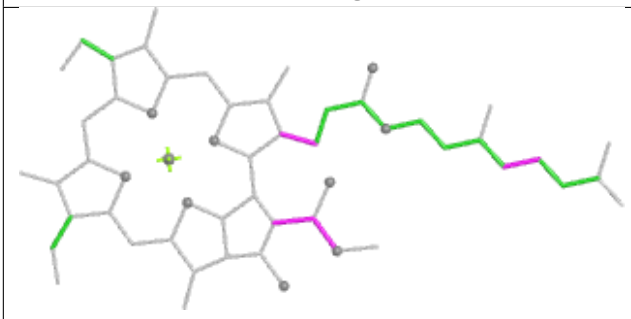
Ligand CLA 2 314



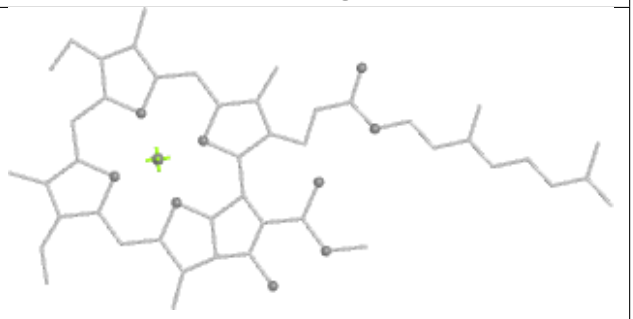
Bond lengths



Bond angles

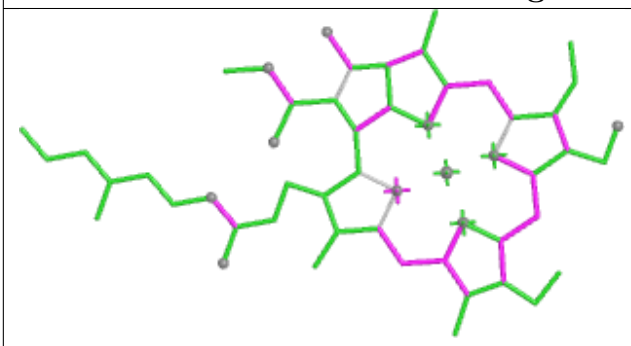


Torsions

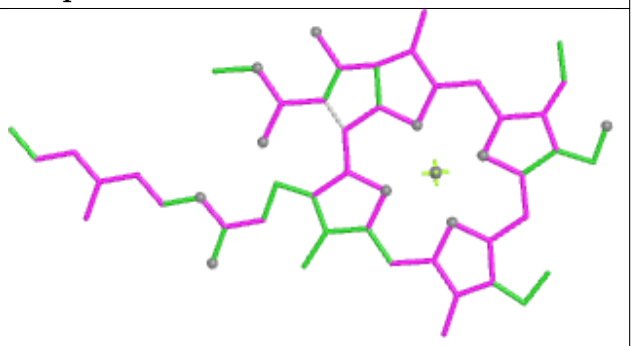


Rings

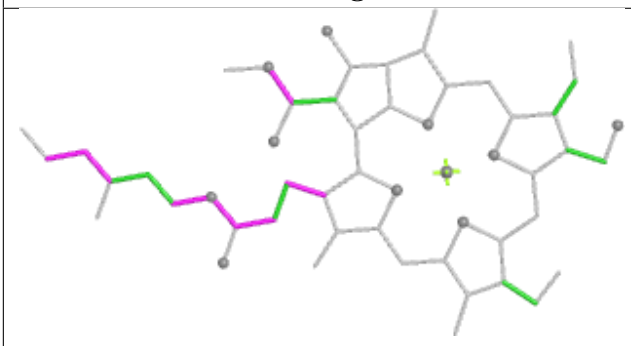
Ligand CHL q 309



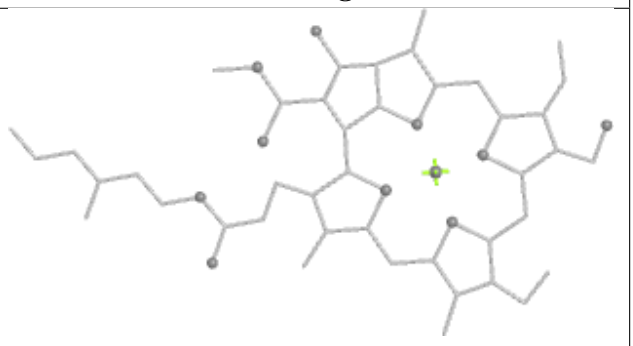
Bond lengths



Bond angles

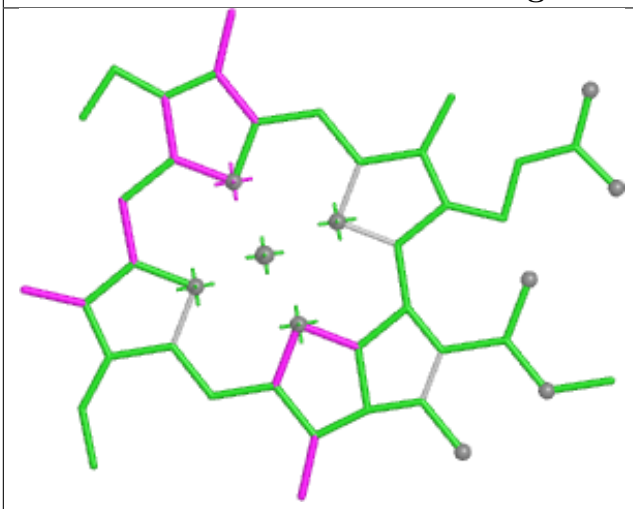


Torsions

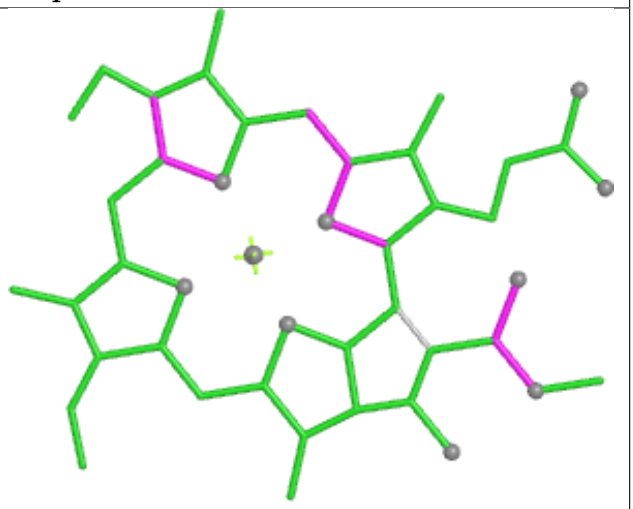


Rings

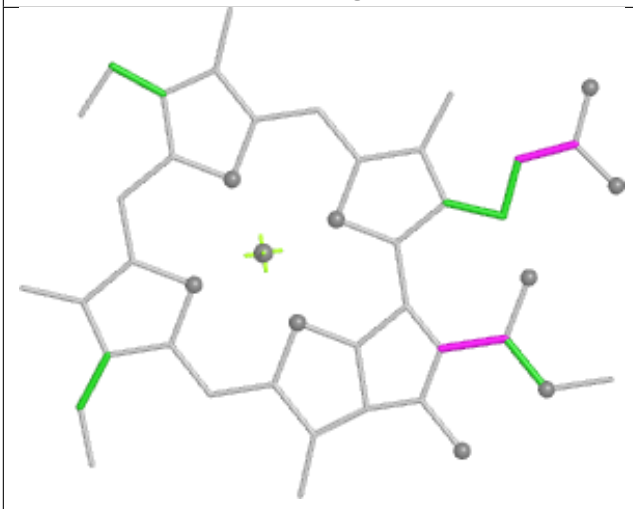
Ligand CLA p 316



Bond lengths



Bond angles

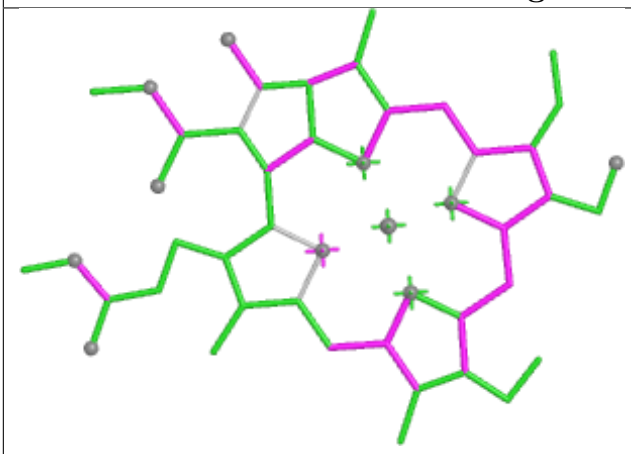


Torsions

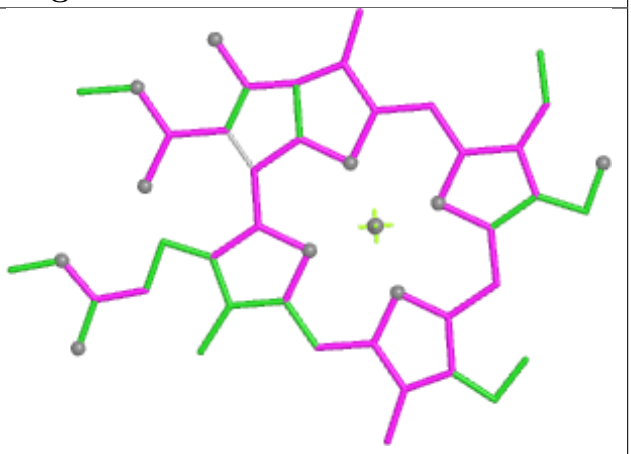


Rings

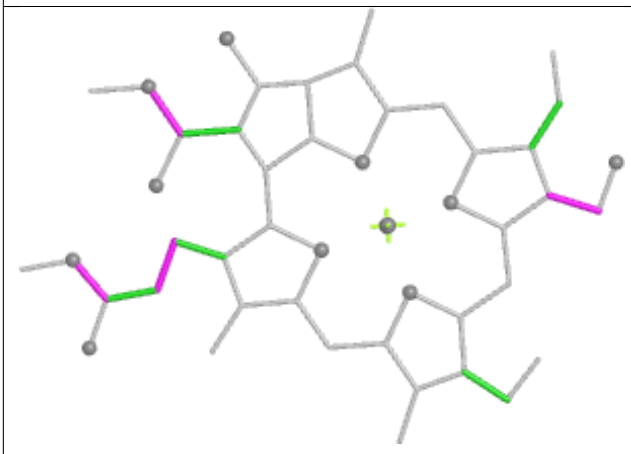
Ligand CHL g 310



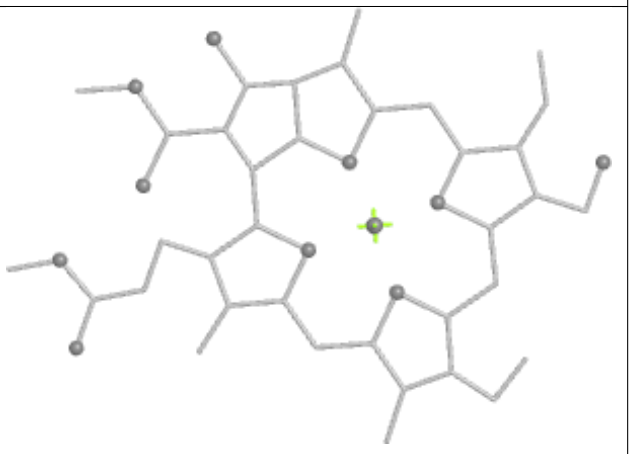
Bond lengths



Bond angles

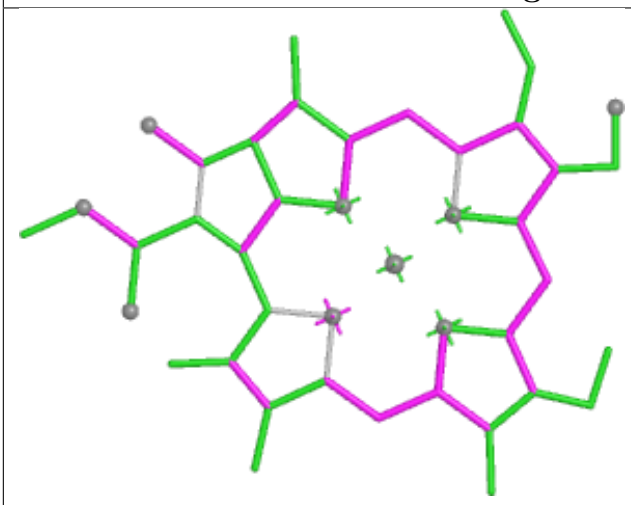


Torsions

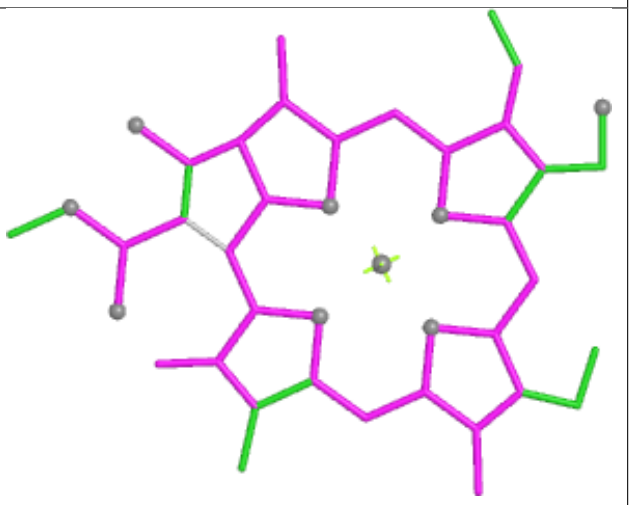


Rings

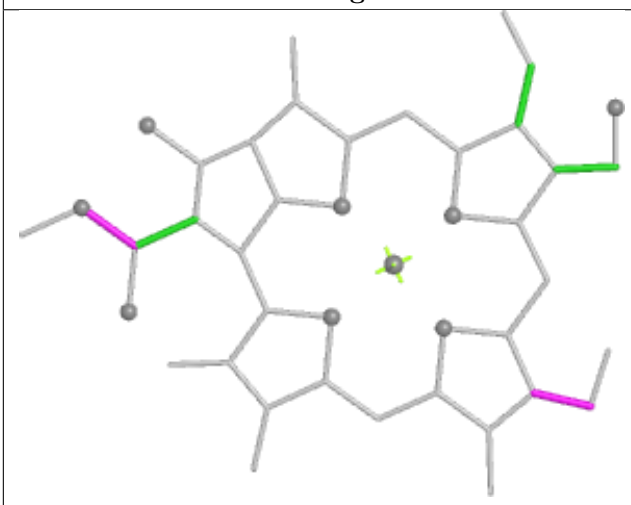
Ligand CHL R 605



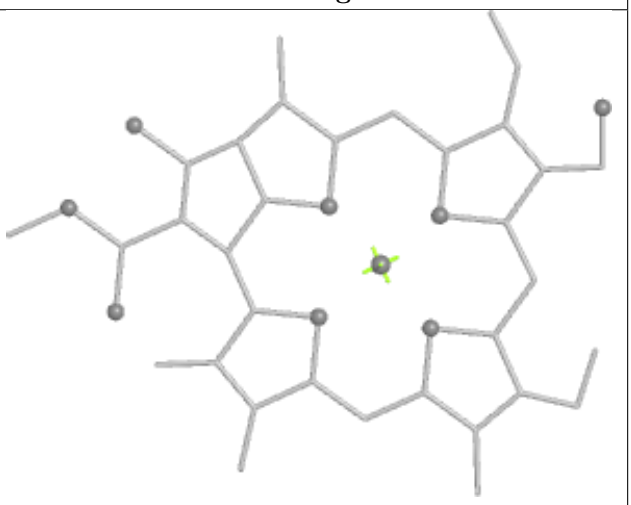
Bond lengths



Bond angles

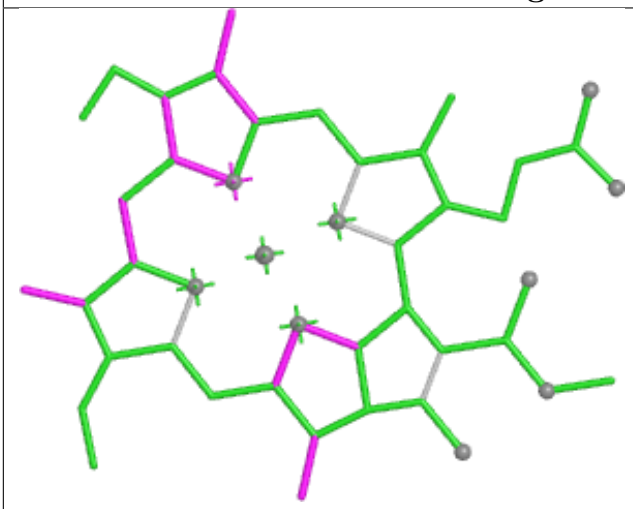


Torsions

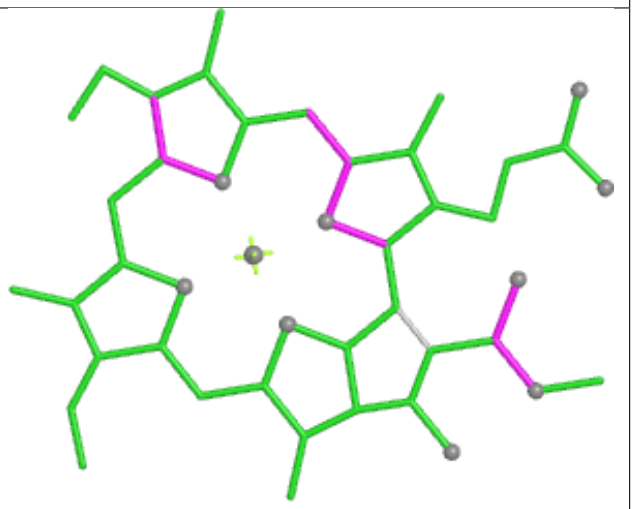


Rings

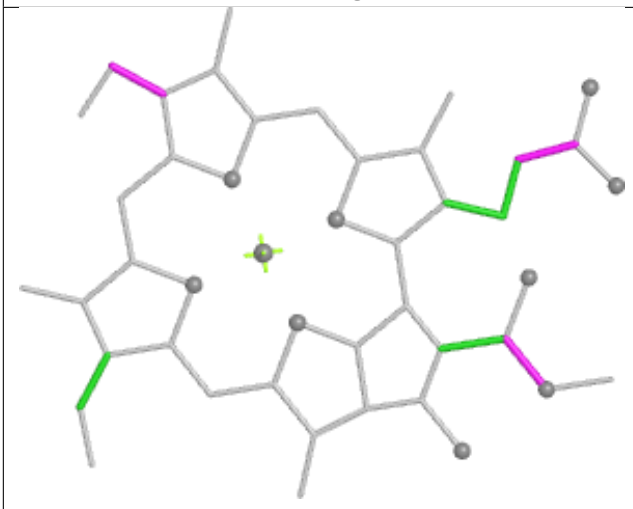
Ligand CLA n 315



Bond lengths



Bond angles

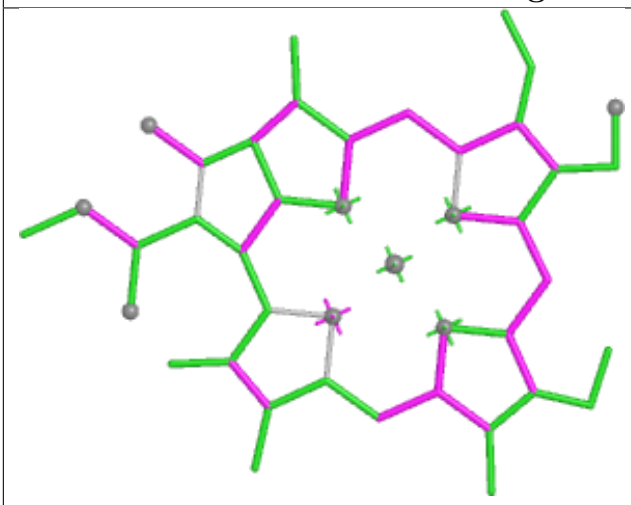


Torsions

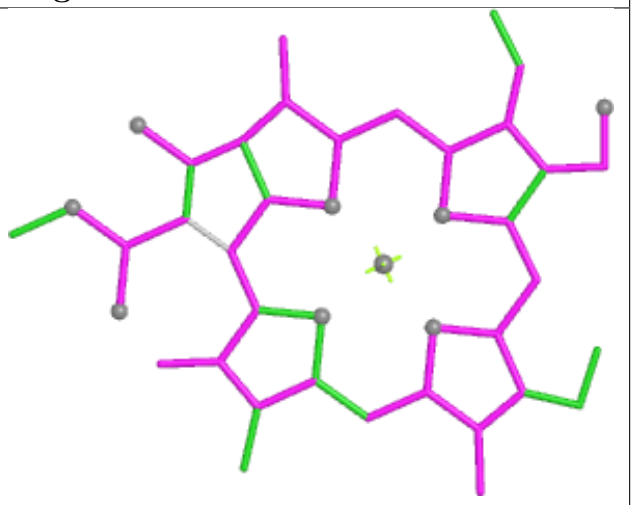


Rings

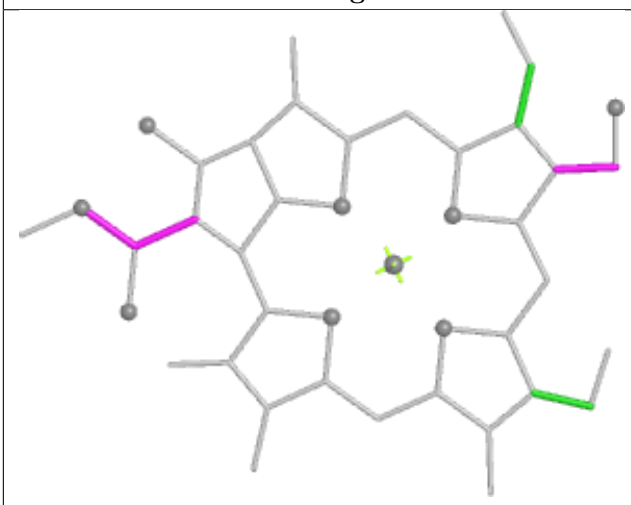
Ligand CHL g 318



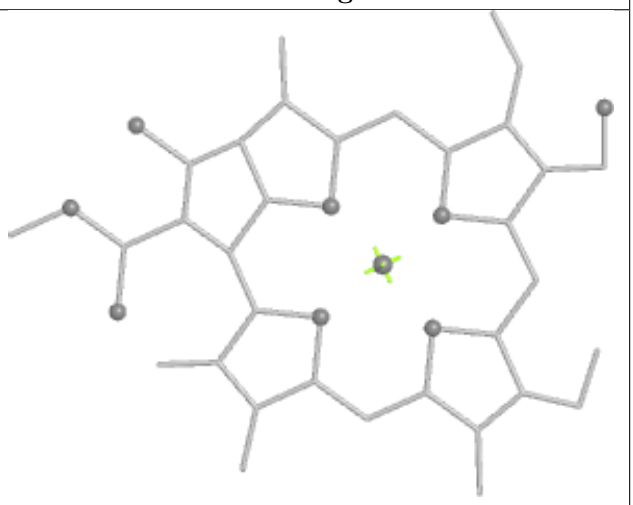
Bond lengths



Bond angles

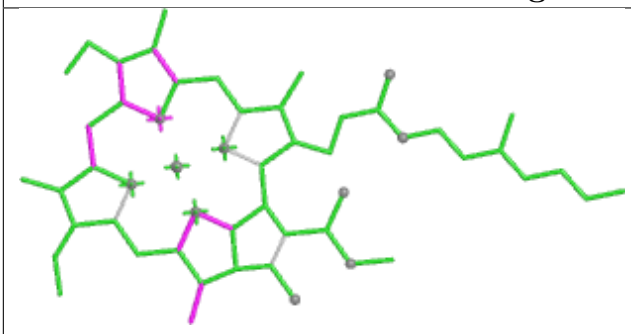


Torsions

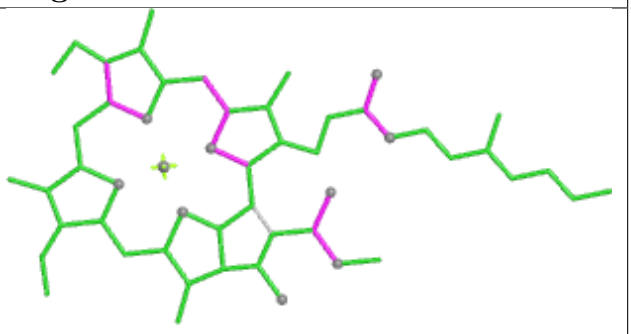


Rings

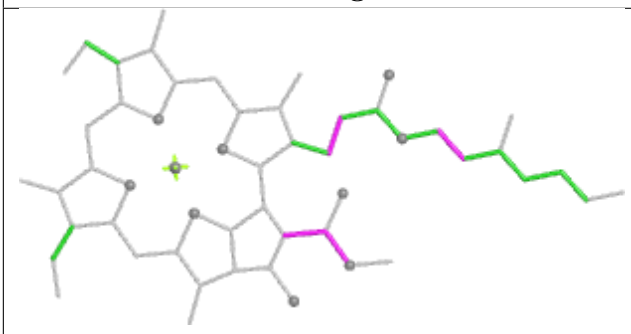
Ligand CLA g 307



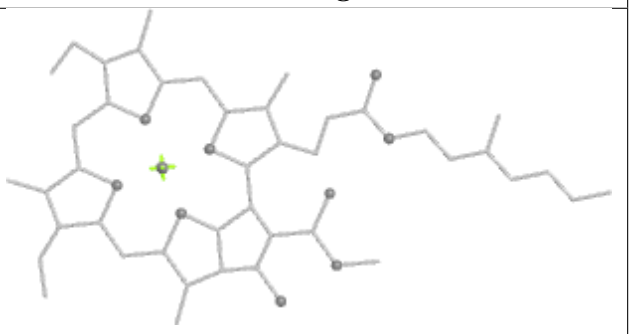
Bond lengths



Bond angles

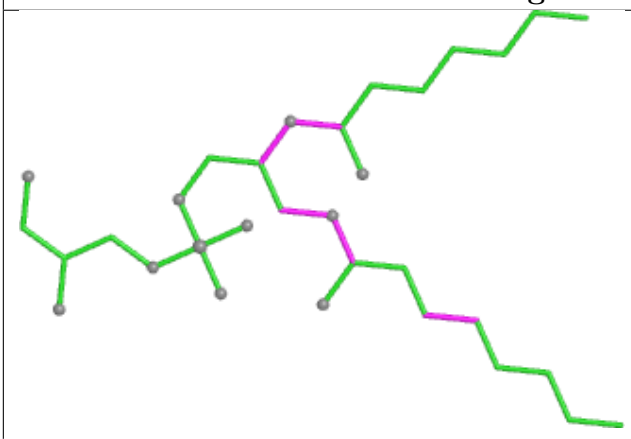


Torsions

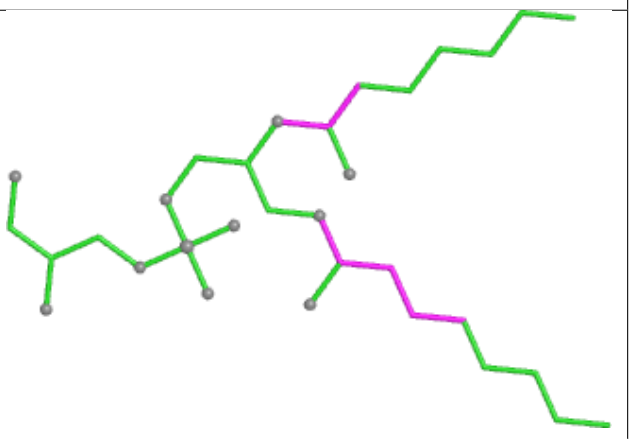


Rings

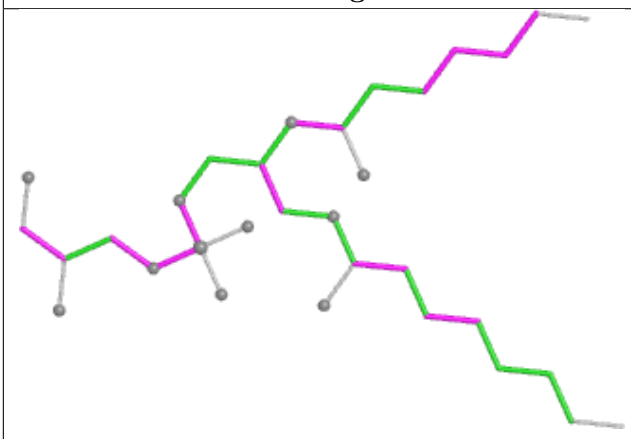
Ligand LHG c 617



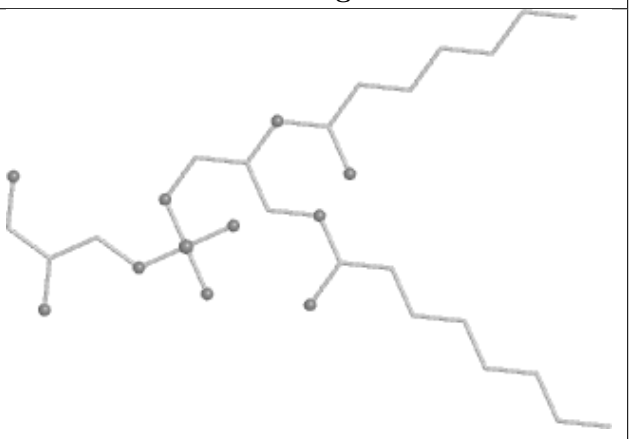
Bond lengths



Bond angles

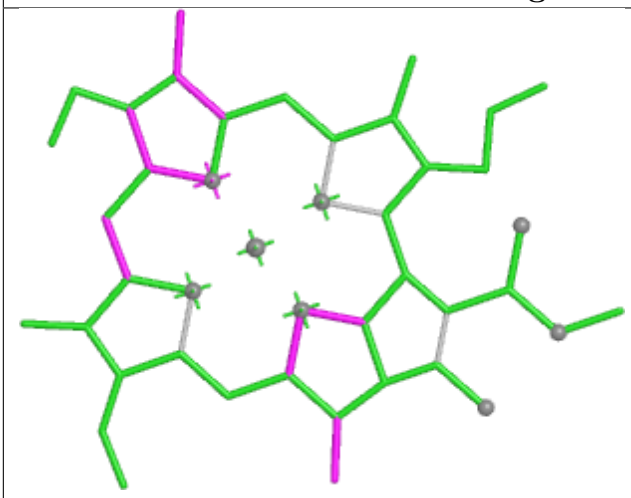


Torsions

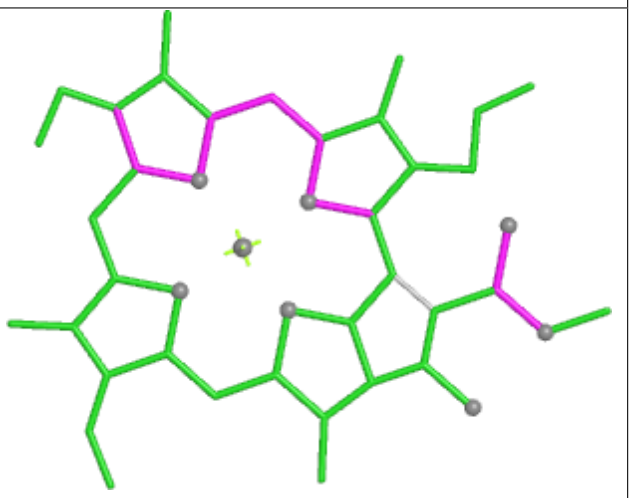


Rings

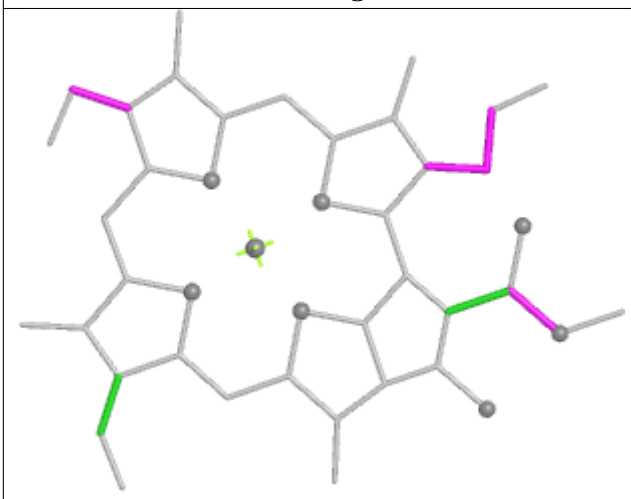
Ligand CLA 2 307



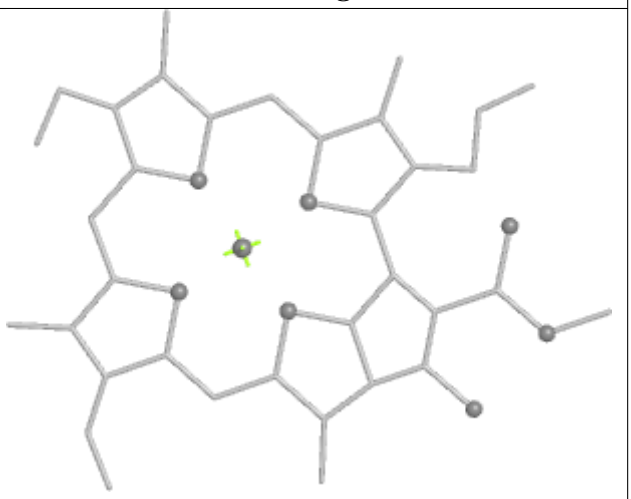
Bond lengths



Bond angles

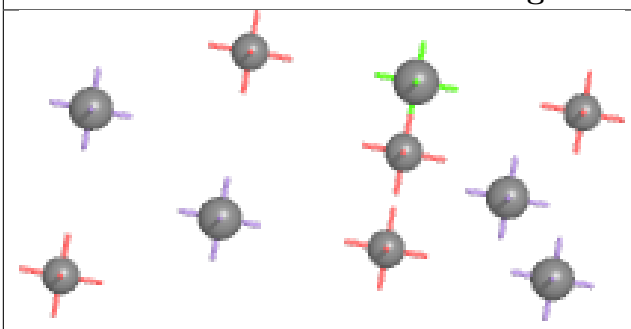


Torsions

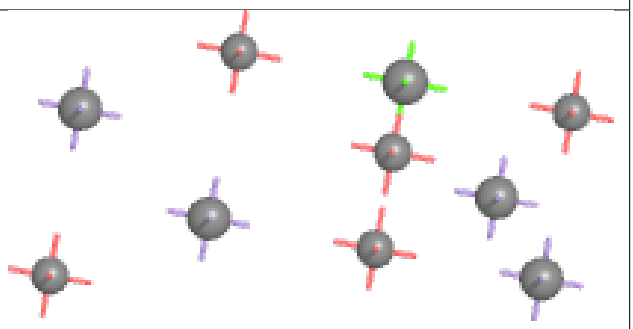


Rings

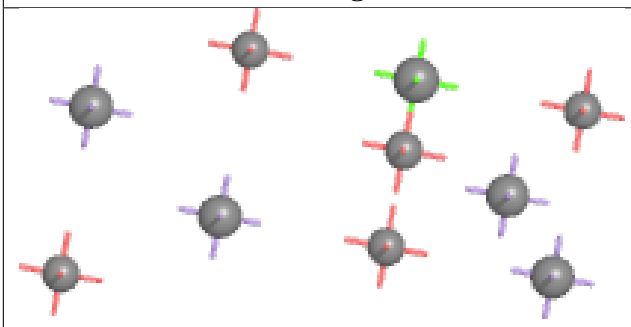
Ligand OEX a 602



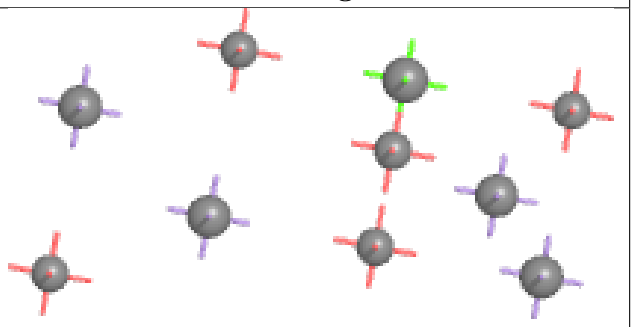
Bond lengths



Bond angles

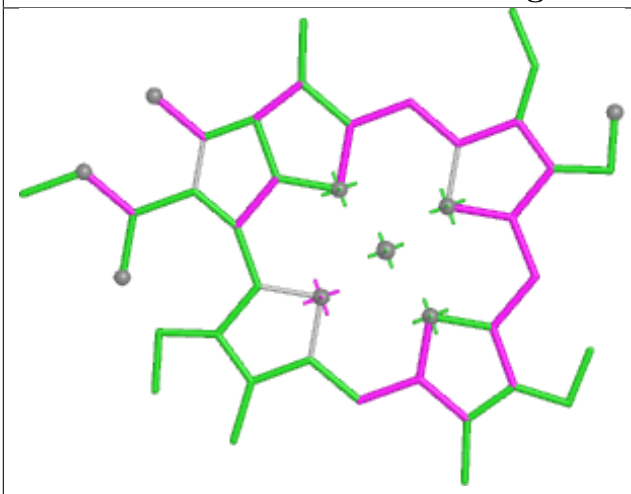


Torsions

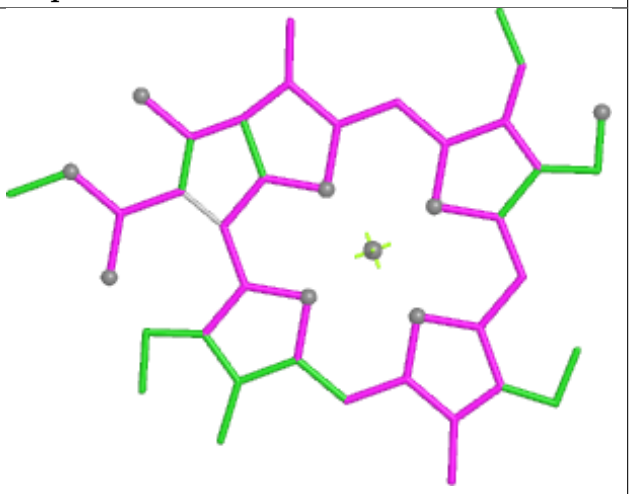


Rings

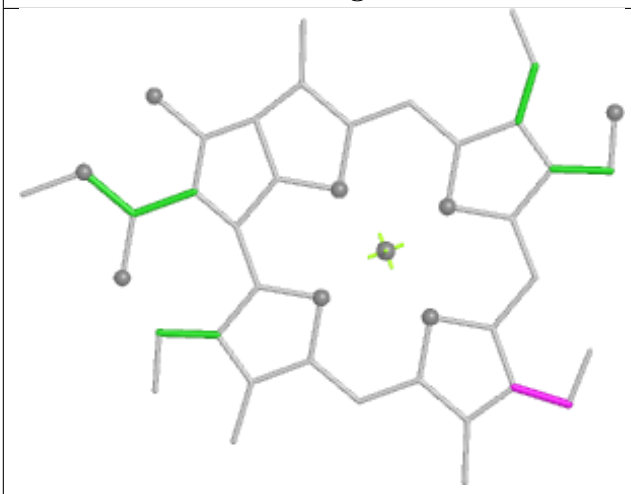
Ligand CHL p 309



Bond lengths



Bond angles

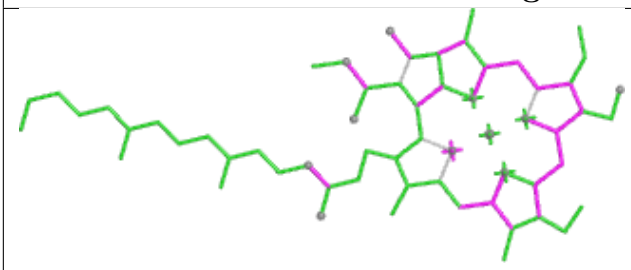


Torsions

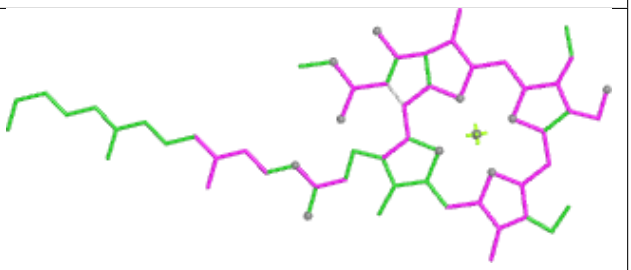


Rings

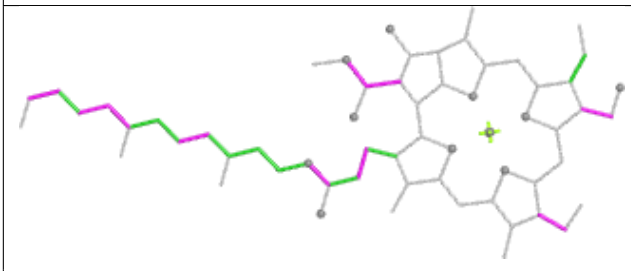
Ligand CHL N 305



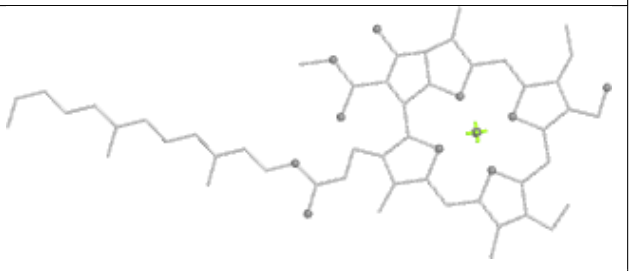
Bond lengths



Bond angles

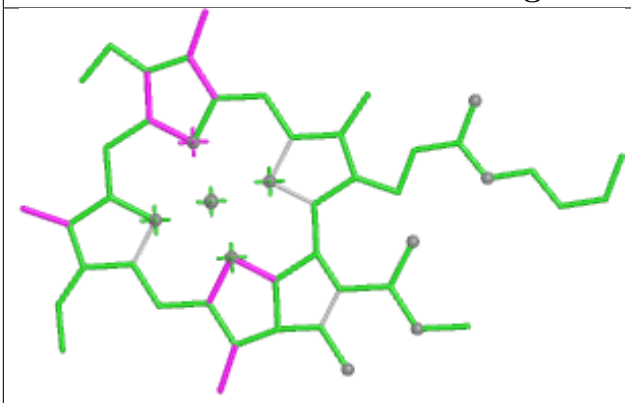


Torsions

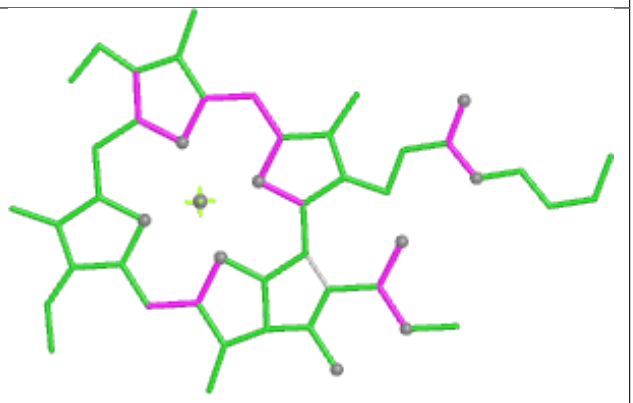


Rings

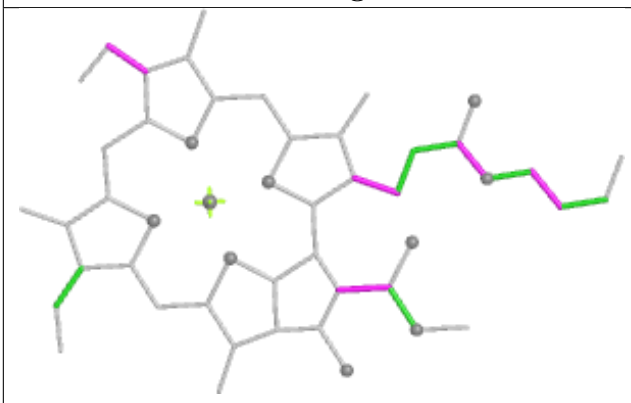
Ligand CLA A 605



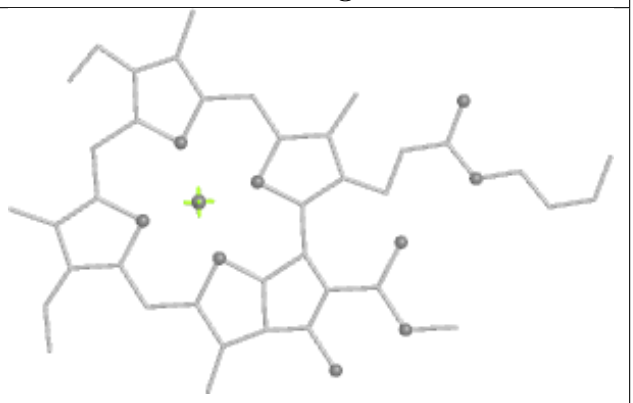
Bond lengths



Bond angles

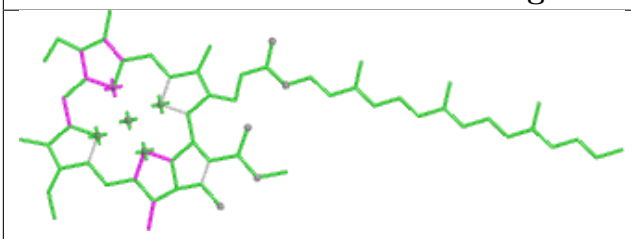


Torsions

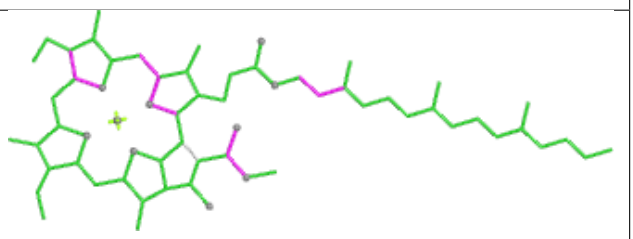


Rings

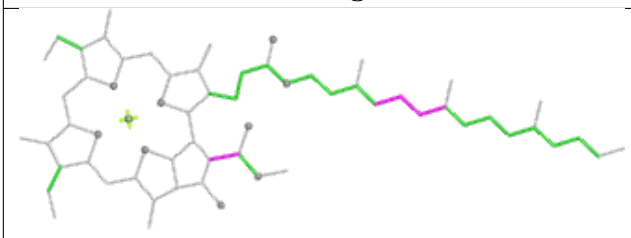
Ligand CLA n 314



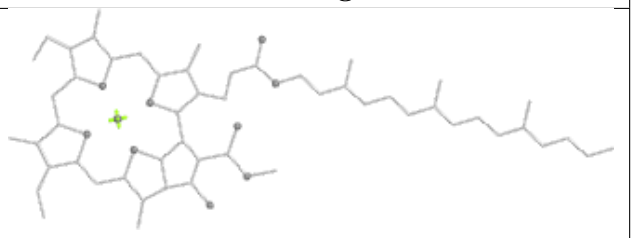
Bond lengths



Bond angles

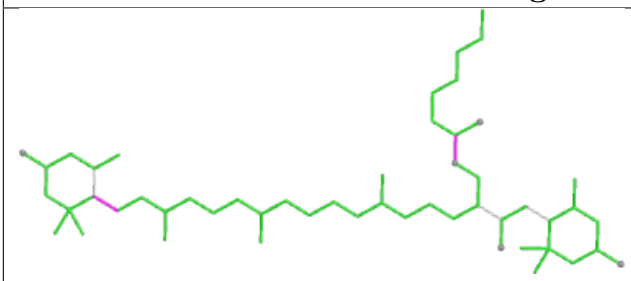


Torsions

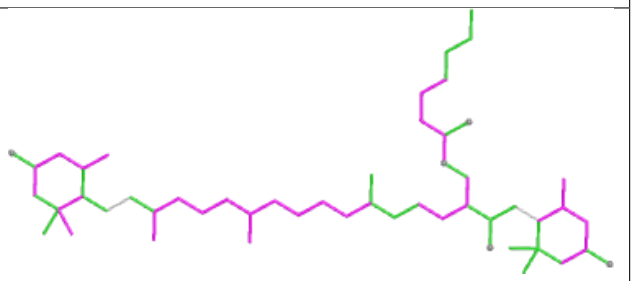


Rings

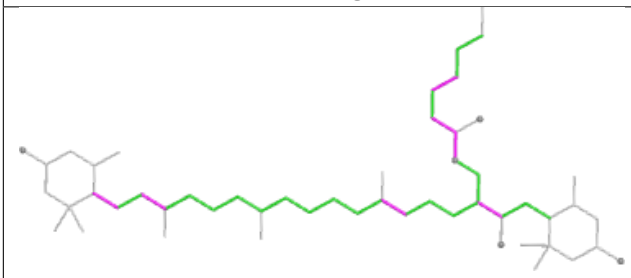
Ligand 0UR 1 301



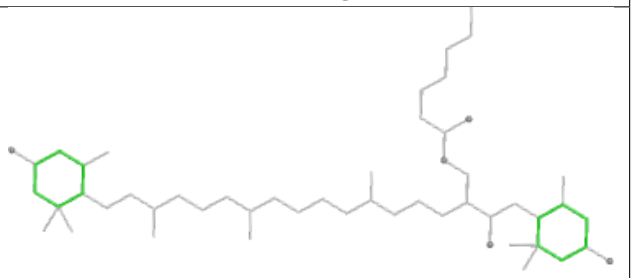
Bond lengths



Bond angles

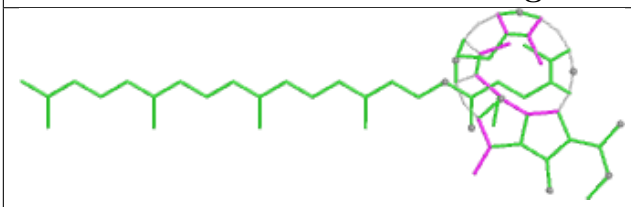


Torsions

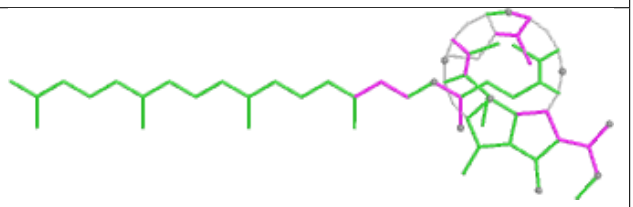


Rings

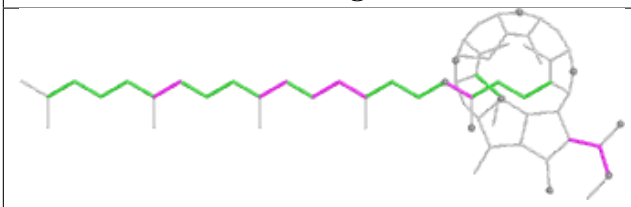
Ligand PHO d 403



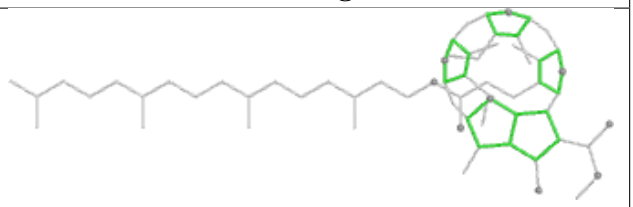
Bond lengths



Bond angles

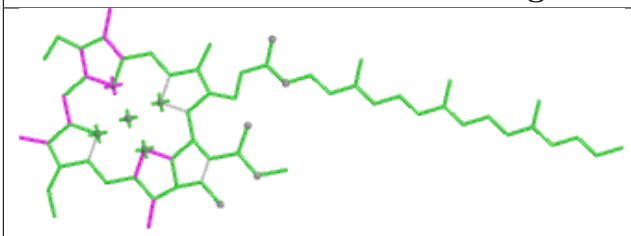


Torsions

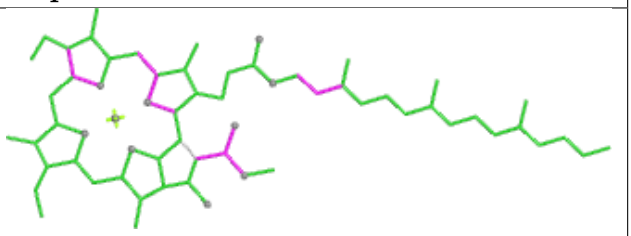


Rings

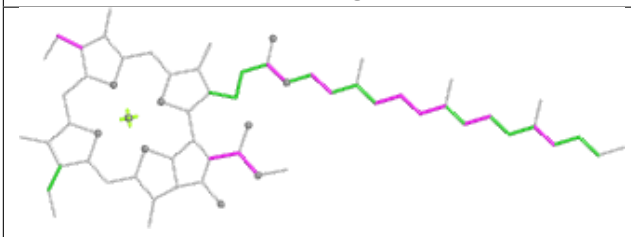
Ligand CLA p 315



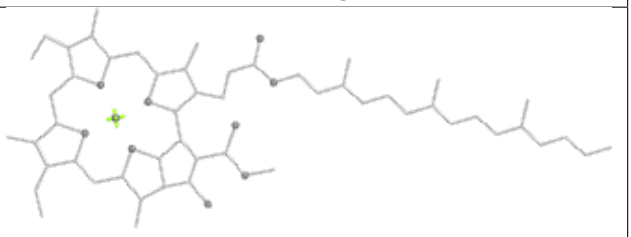
Bond lengths



Bond angles

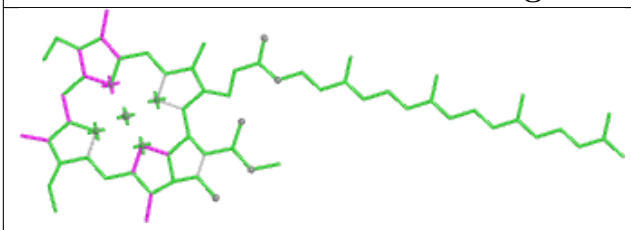


Torsions

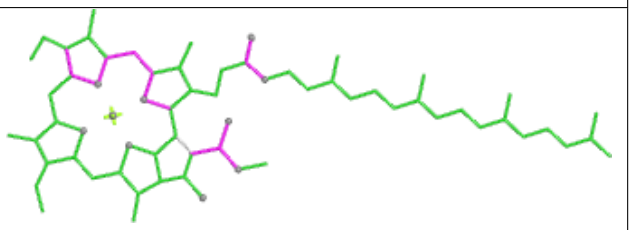


Rings

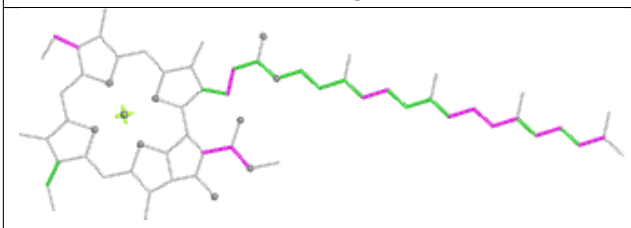
Ligand CLA B 607



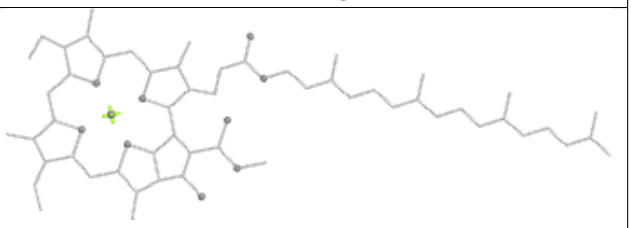
Bond lengths



Bond angles

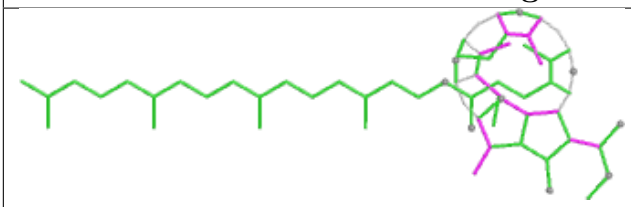


Torsions

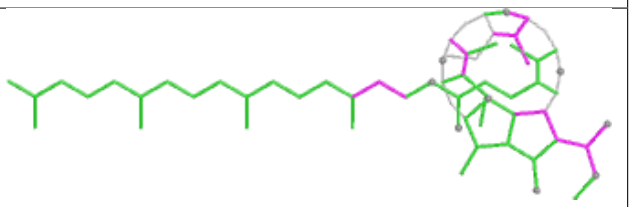


Rings

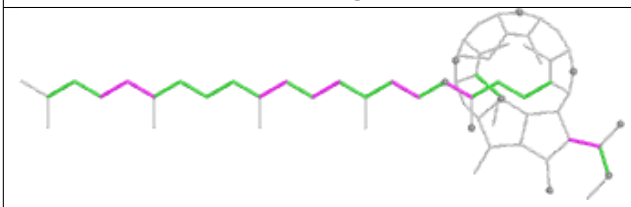
Ligand PHO A 606



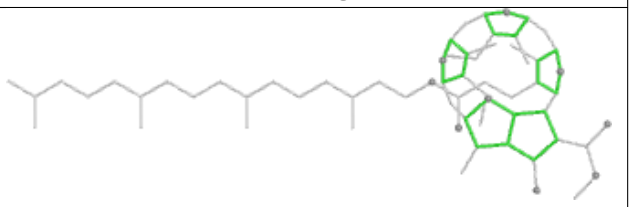
Bond lengths



Bond angles

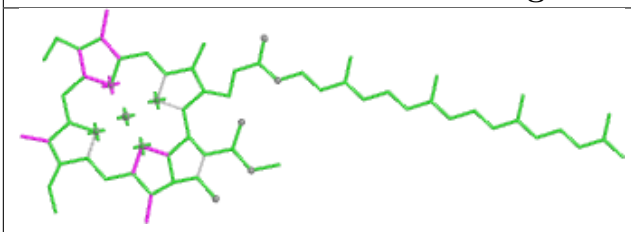


Torsions

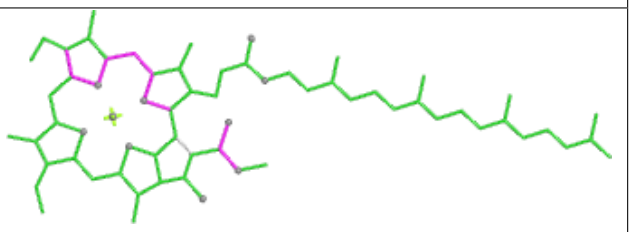


Rings

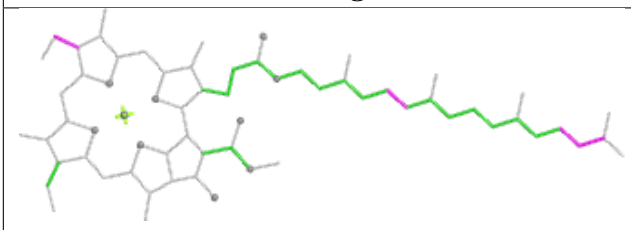
Ligand CLA b 615



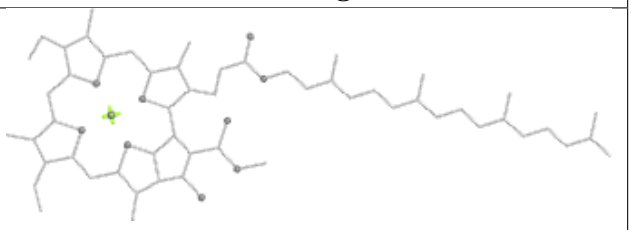
Bond lengths



Bond angles

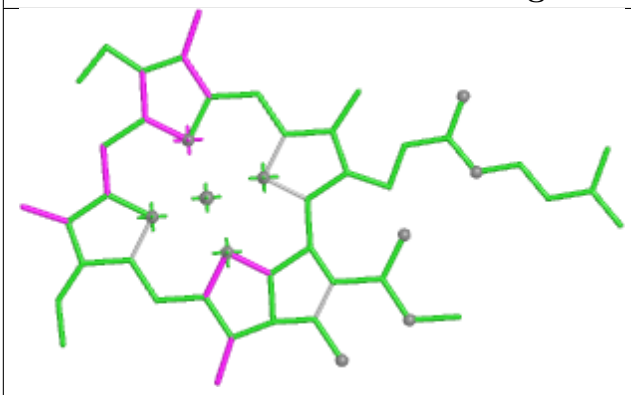


Torsions

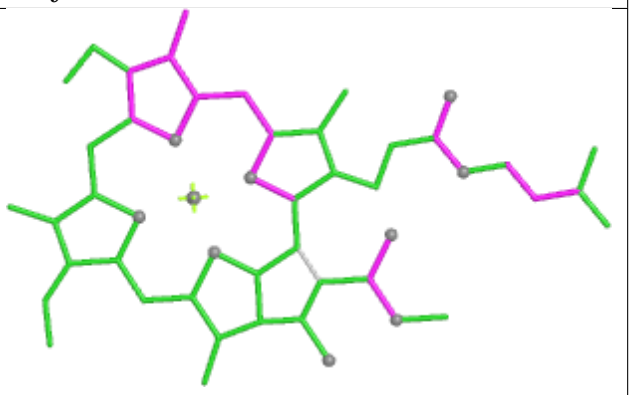


Rings

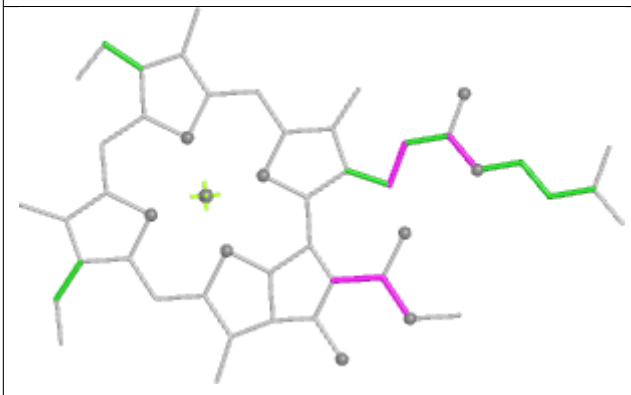
Ligand CLA y 308



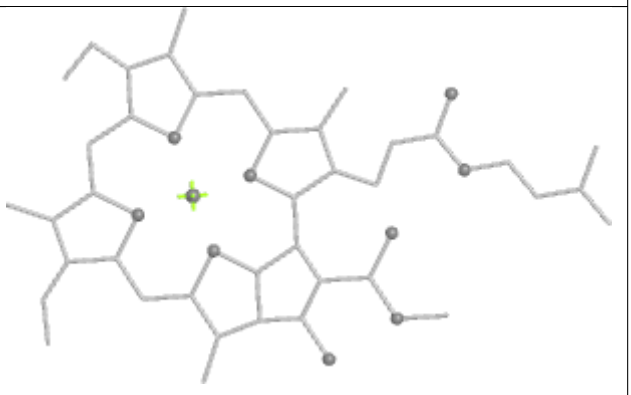
Bond lengths



Bond angles

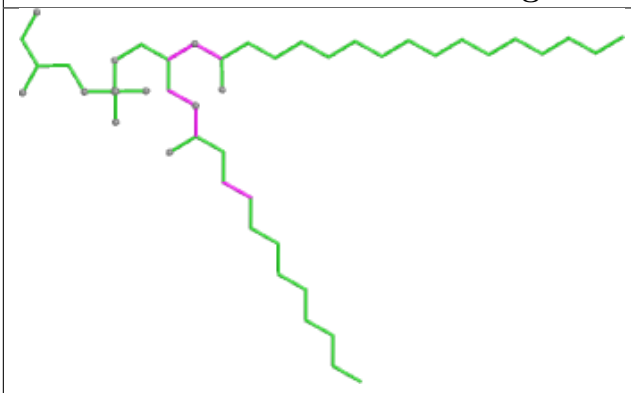


Torsions

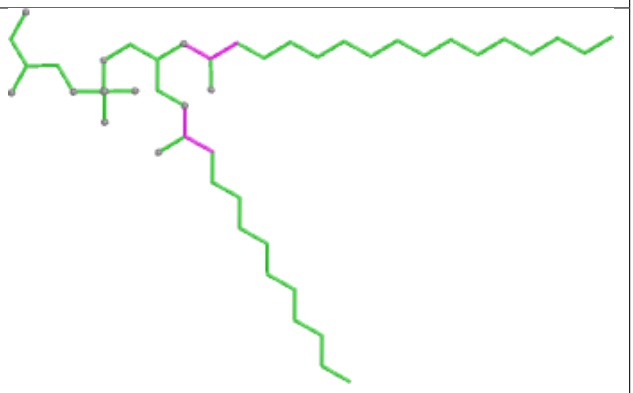


Rings

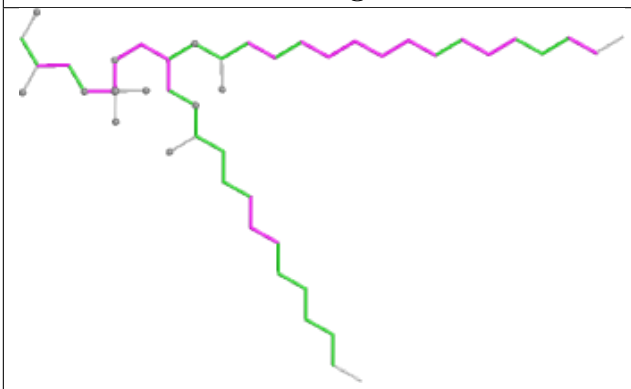
Ligand LHG A 601



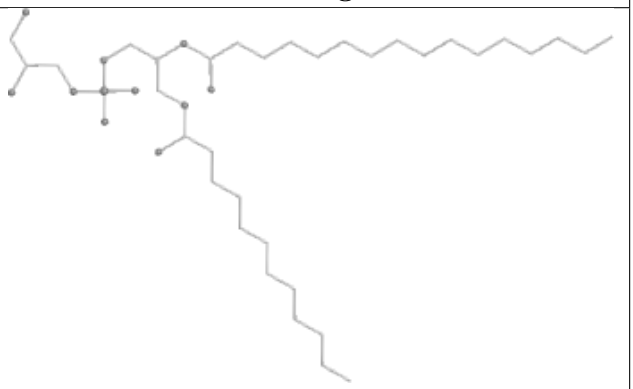
Bond lengths



Bond angles

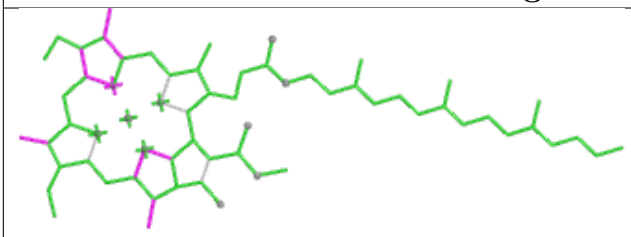


Torsions

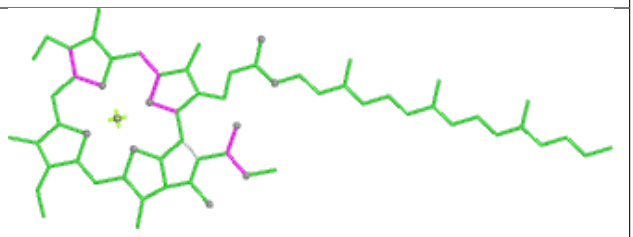


Rings

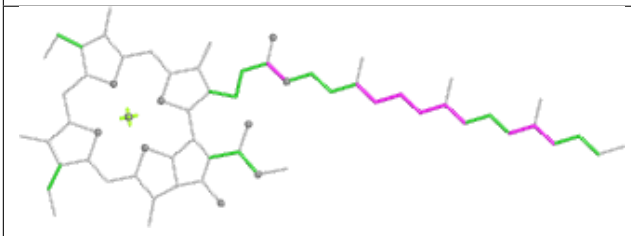
Ligand CLA Y 314



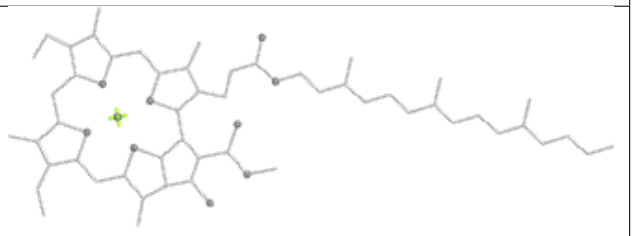
Bond lengths



Bond angles

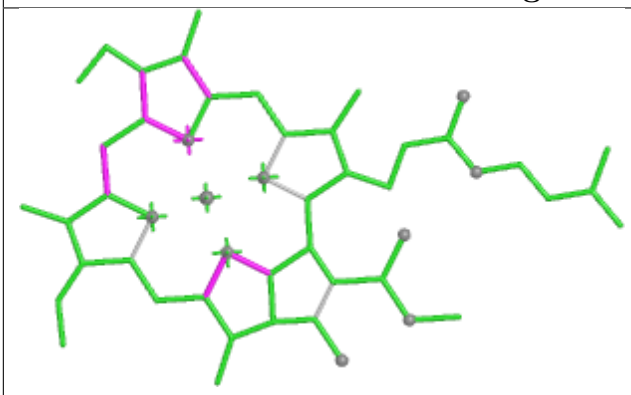


Torsions

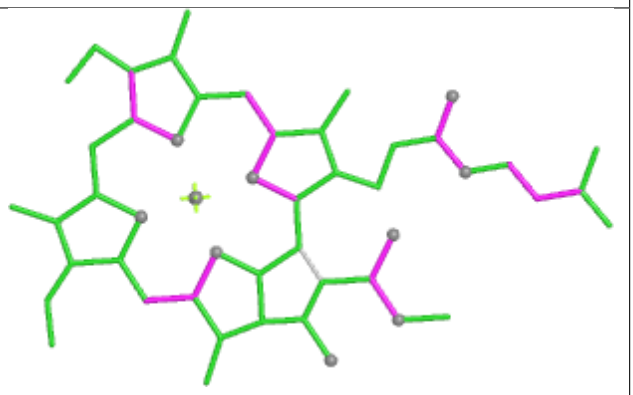


Rings

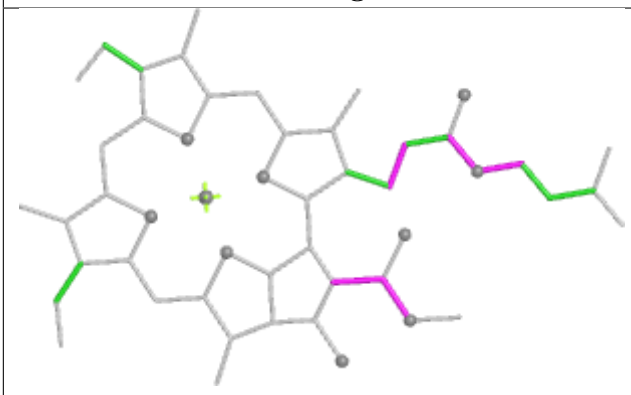
Ligand CLA G 308



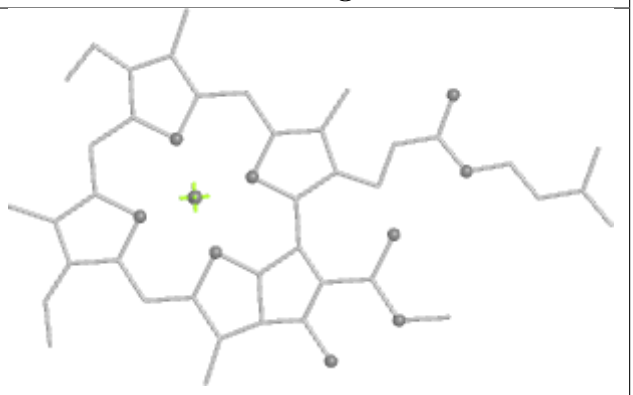
Bond lengths



Bond angles

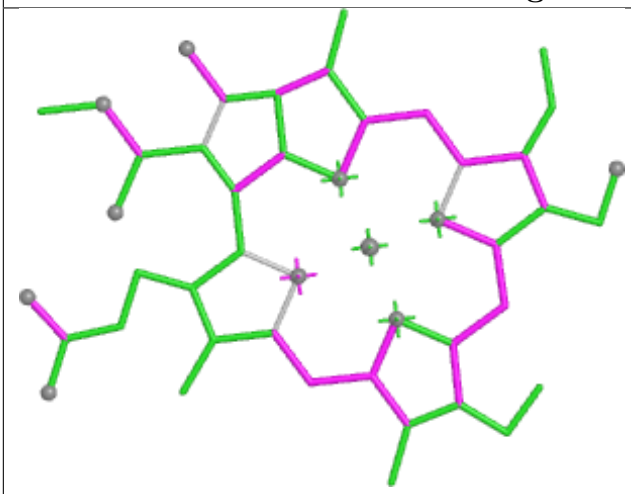


Torsions

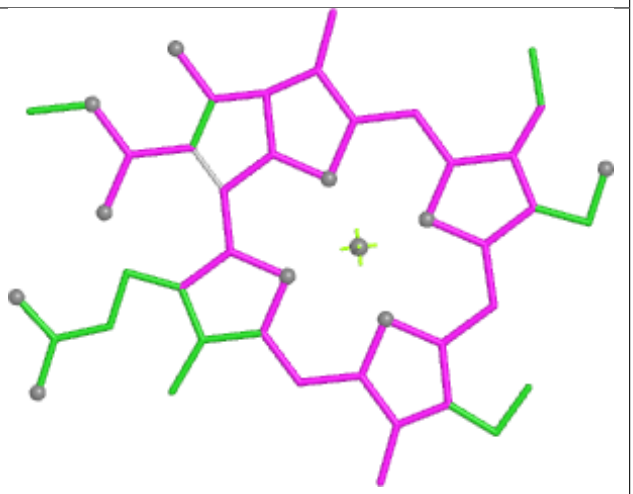


Rings

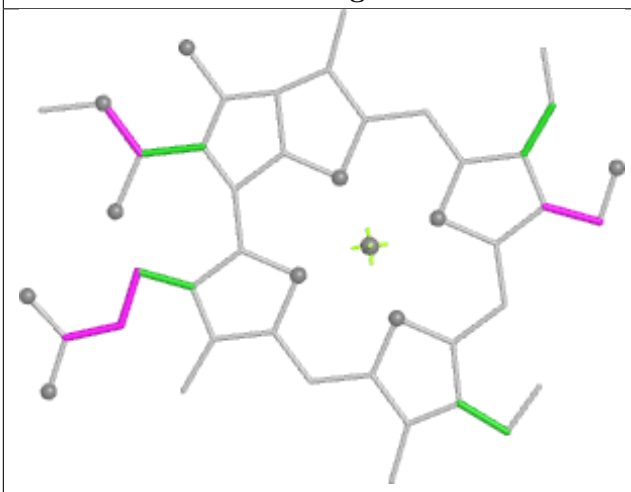
Ligand CHL n 309



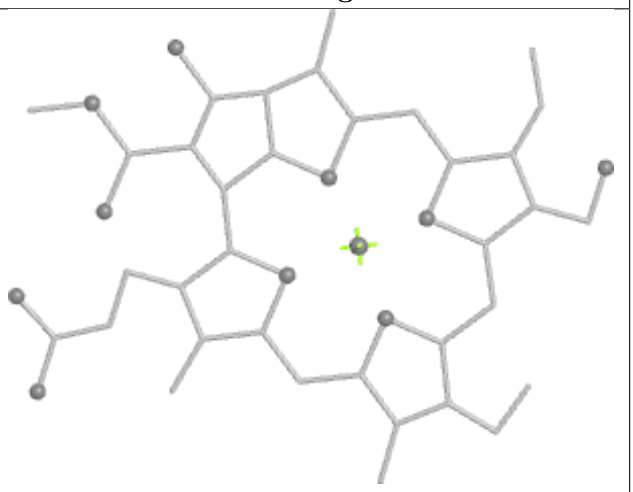
Bond lengths



Bond angles

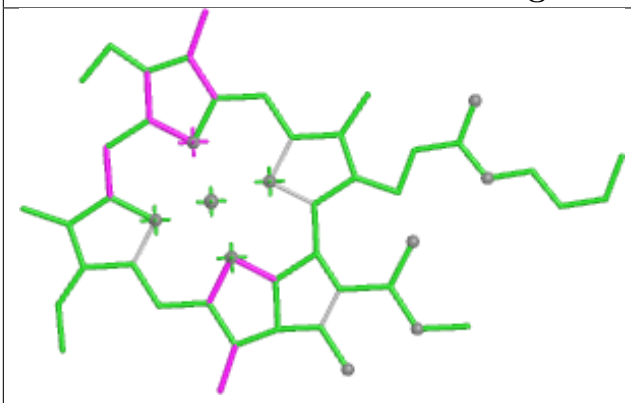


Torsions

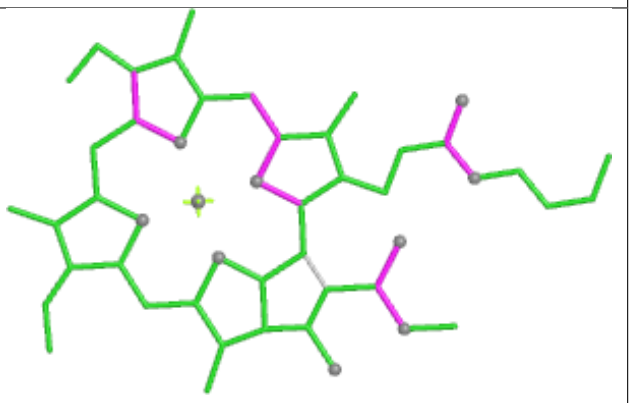


Rings

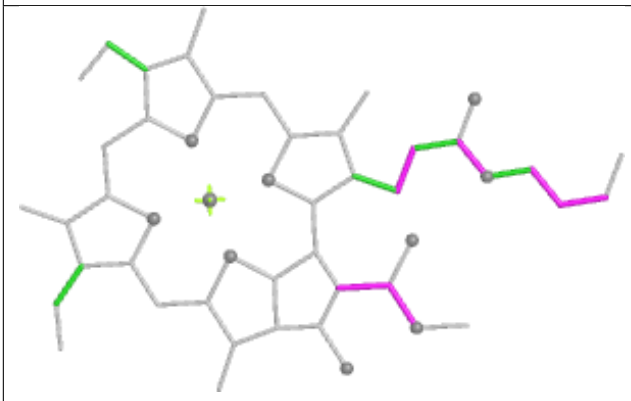
Ligand CLA 2 317



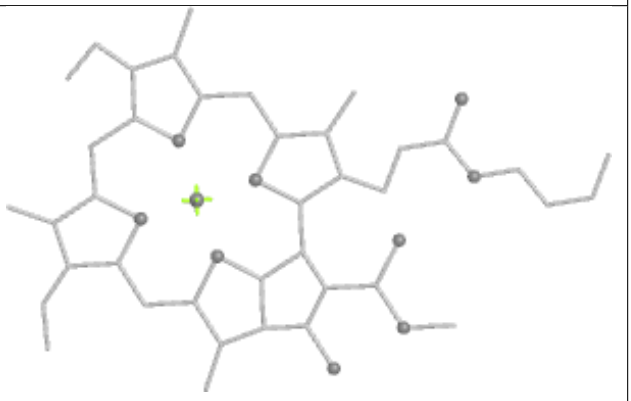
Bond lengths



Bond angles

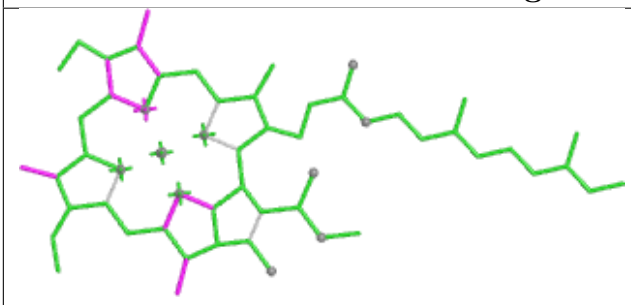


Torsions

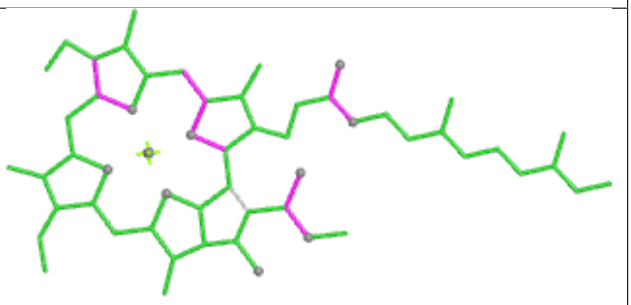


Rings

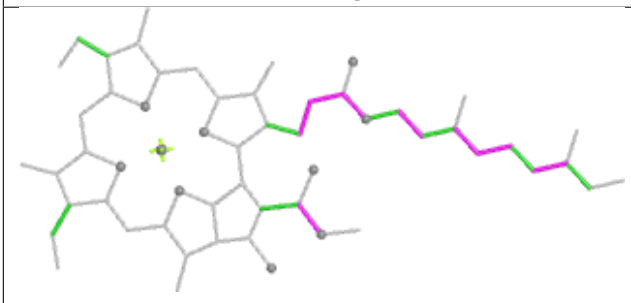
Ligand CLA B 614



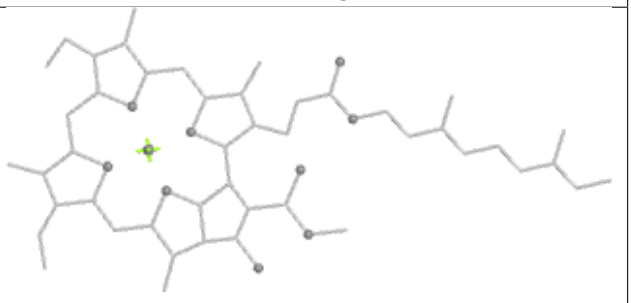
Bond lengths



Bond angles

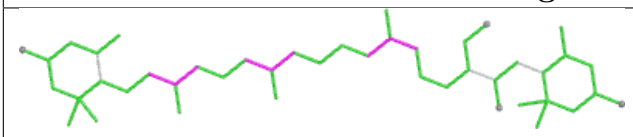


Torsions

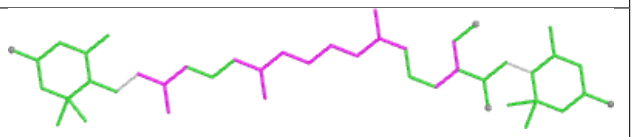


Rings

Ligand 0IE 2 303



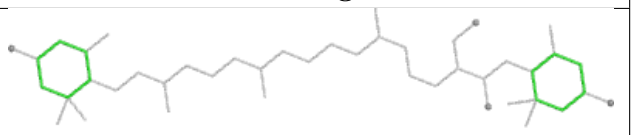
Bond lengths



Bond angles

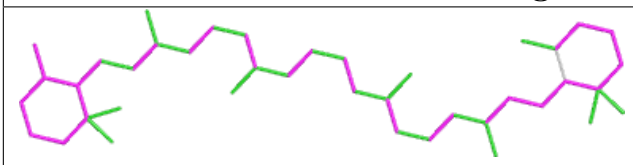


Torsions

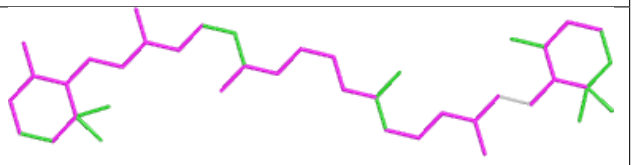


Rings

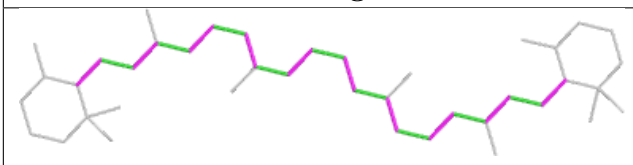
Ligand 8CT c 614



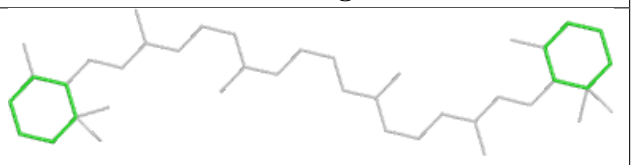
Bond lengths



Bond angles

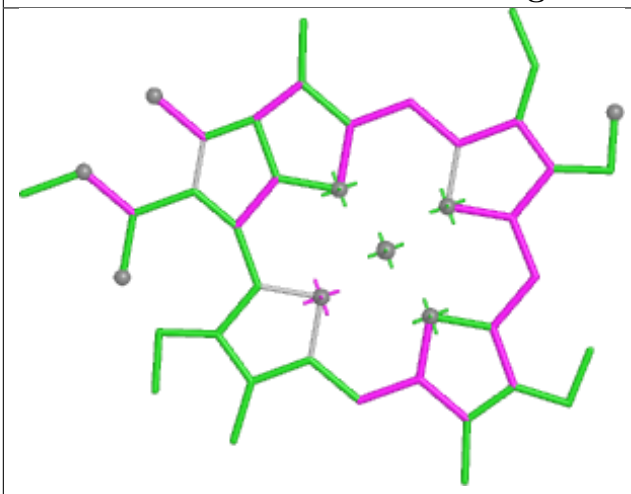


Torsions

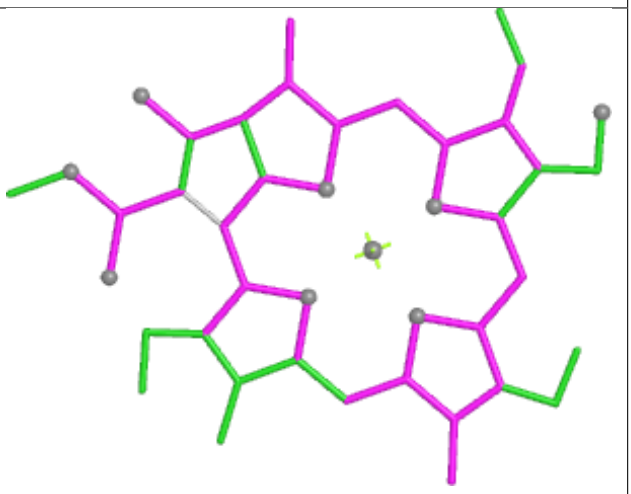


Rings

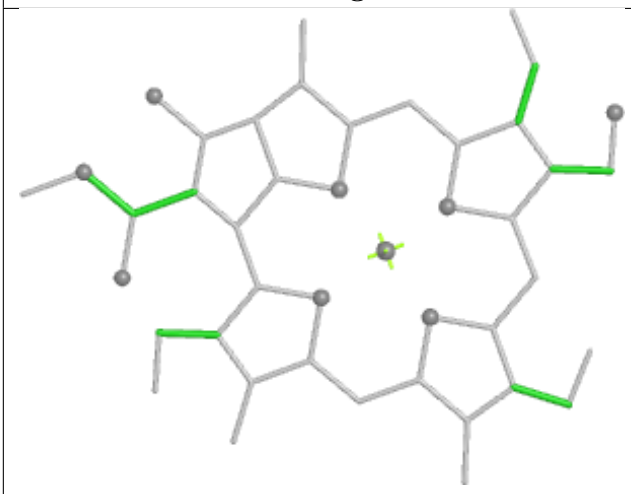
Ligand CHL 7 309



Bond lengths



Bond angles

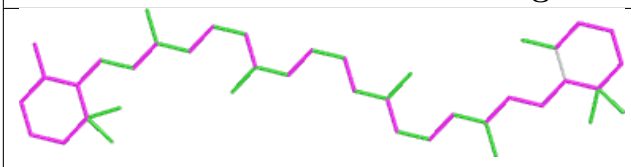


Torsions

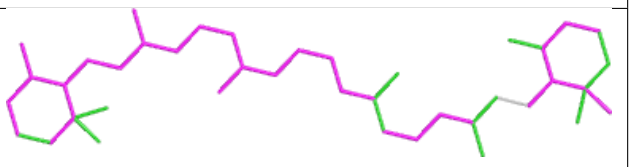


Rings

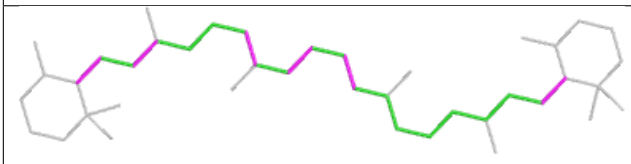
Ligand 8CT c 613



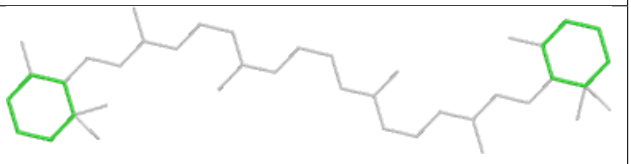
Bond lengths



Bond angles

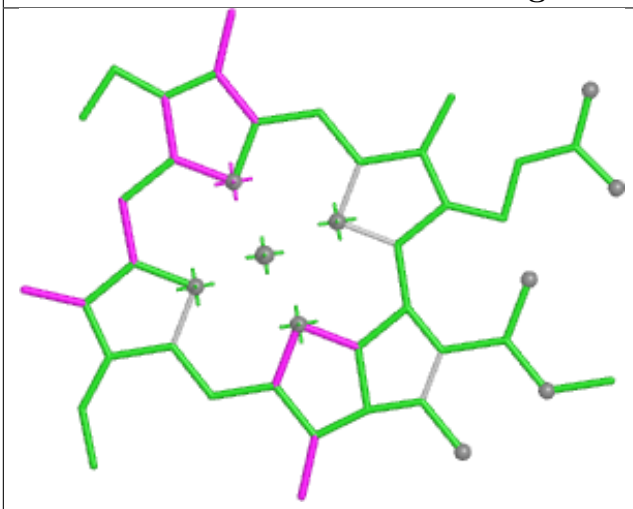


Torsions

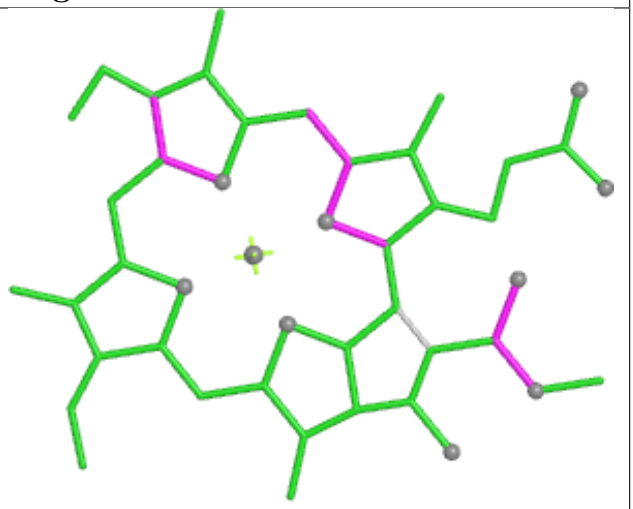


Rings

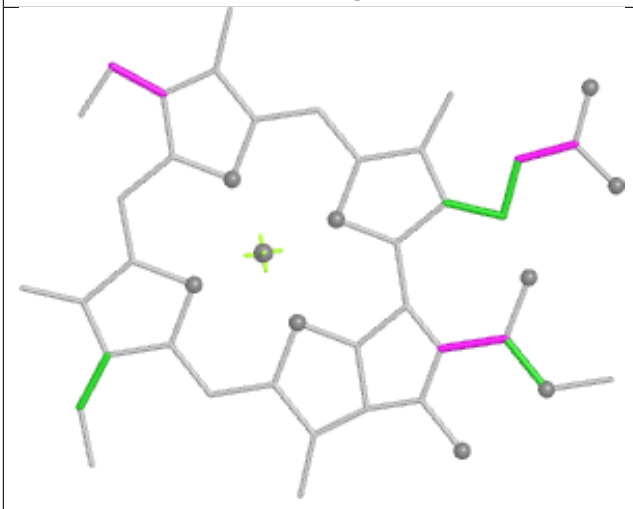
Ligand CLA g 316



Bond lengths



Bond angles

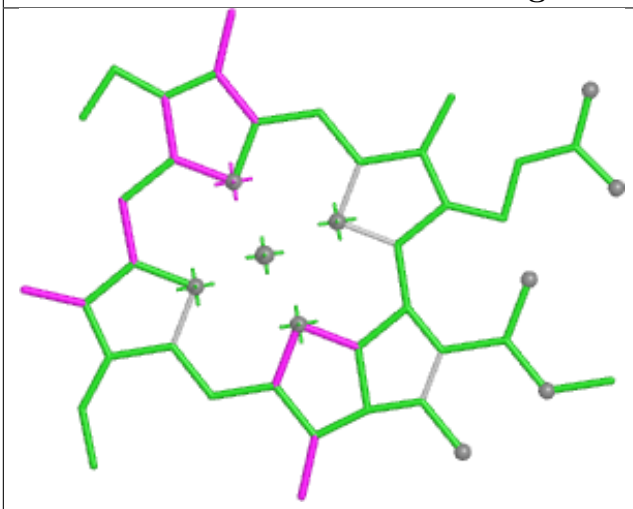


Torsions

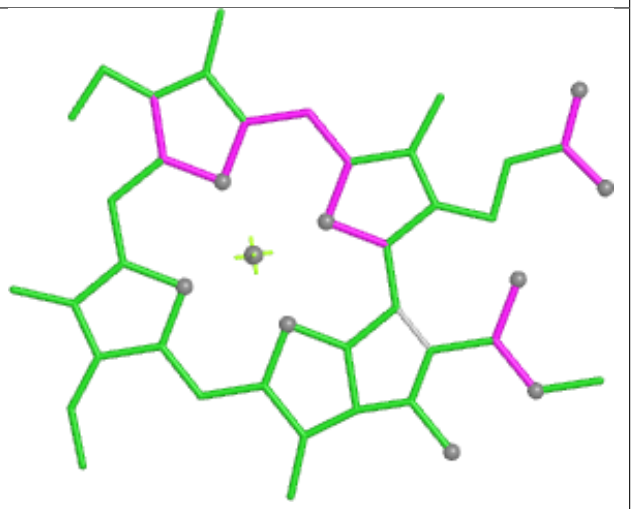


Rings

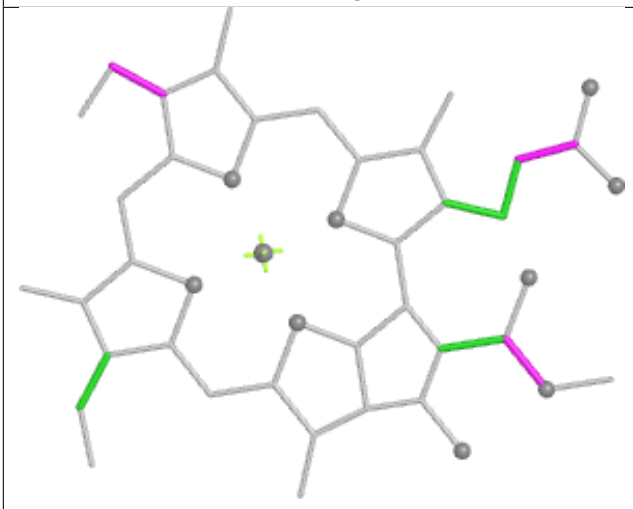
Ligand CLA 3 315



Bond lengths



Bond angles

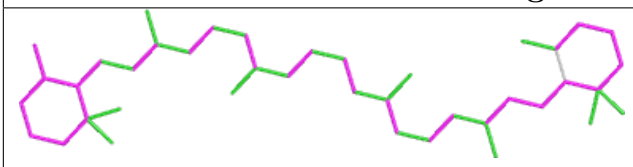


Torsions

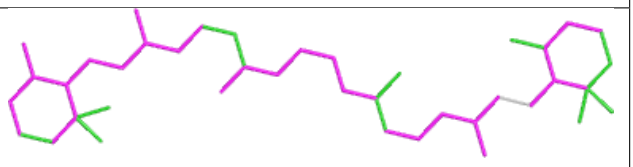


Rings

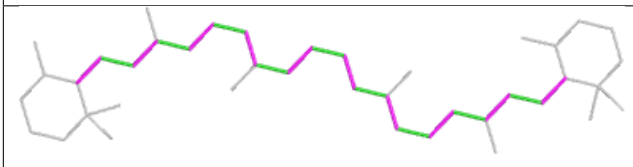
Ligand 8CT C 614



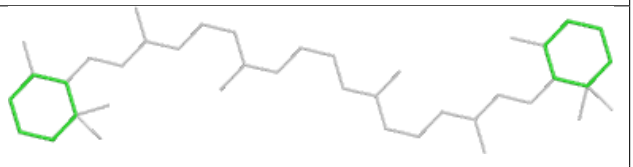
Bond lengths



Bond angles

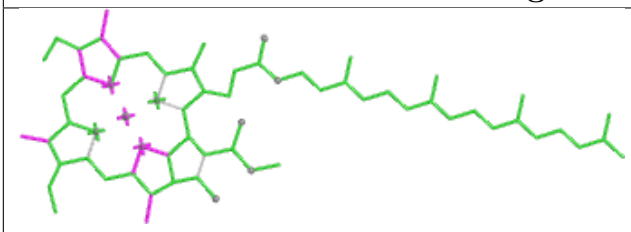


Torsions

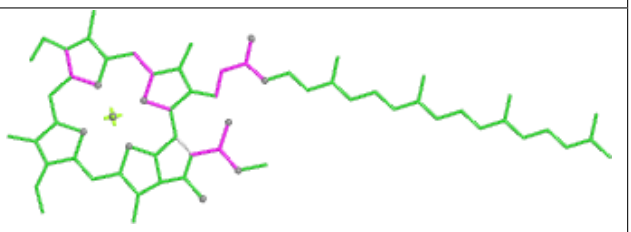


Rings

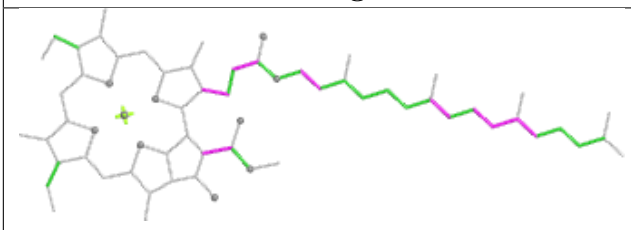
Ligand CLA d 404



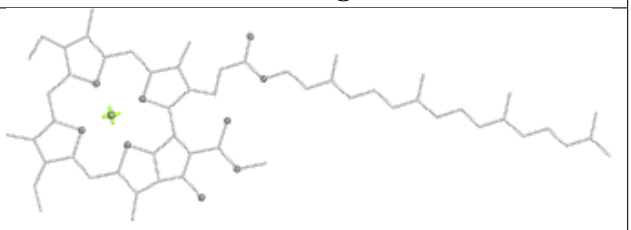
Bond lengths



Bond angles



Torsions



Rings

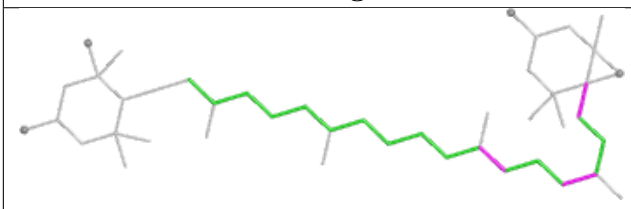
Ligand NEX r 317



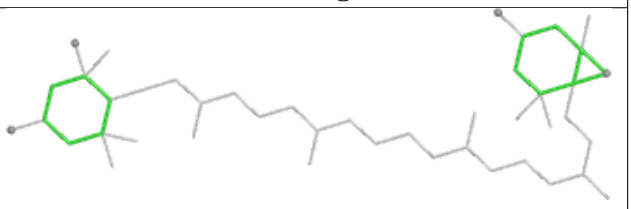
Bond lengths



Bond angles

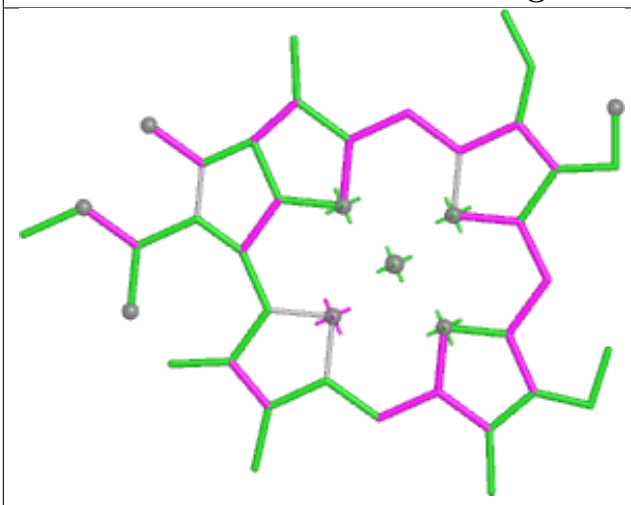


Torsions

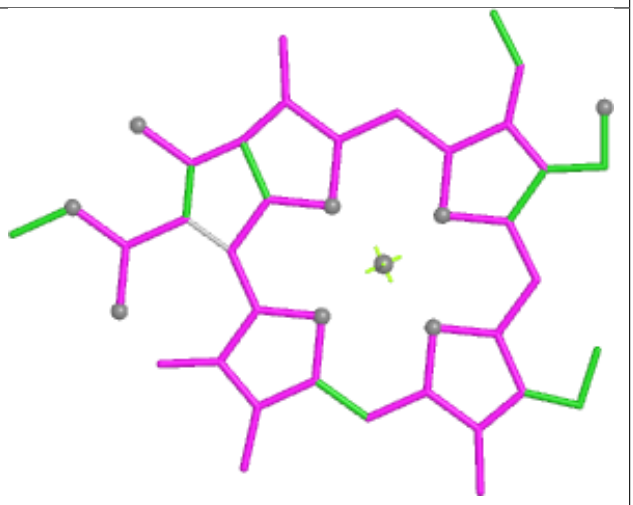


Rings

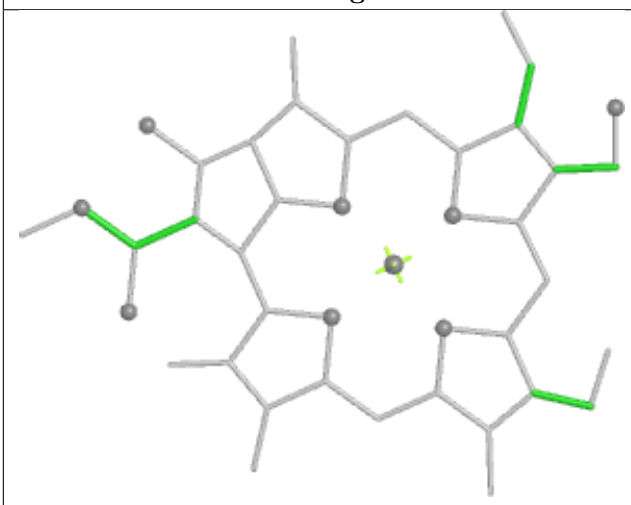
Ligand CHL 6 317



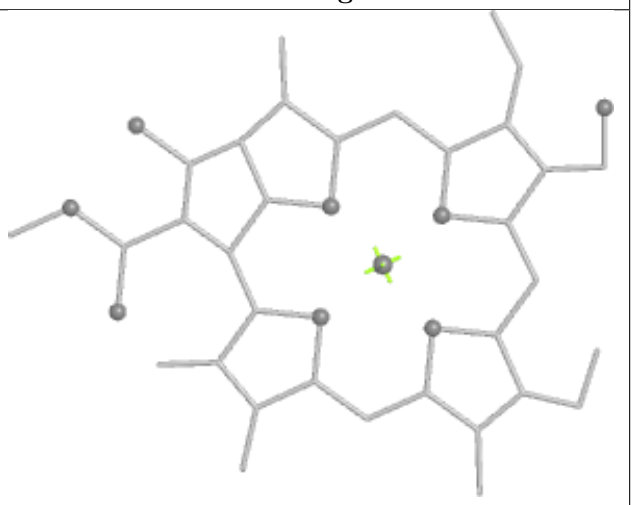
Bond lengths



Bond angles

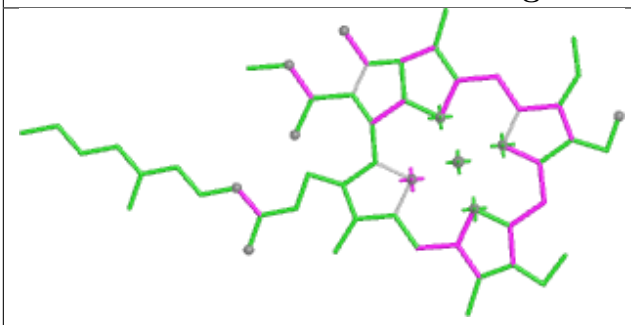


Torsions

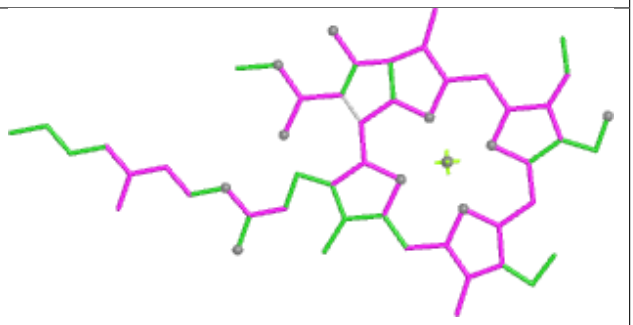


Rings

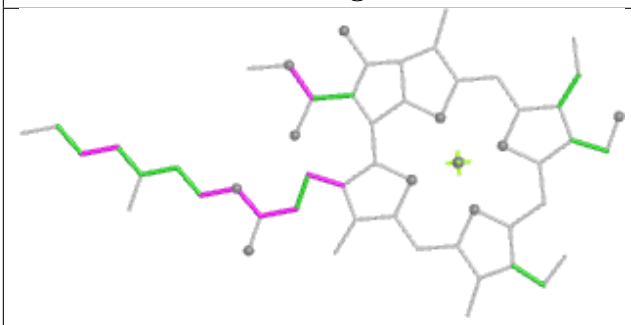
Ligand CHL G 311



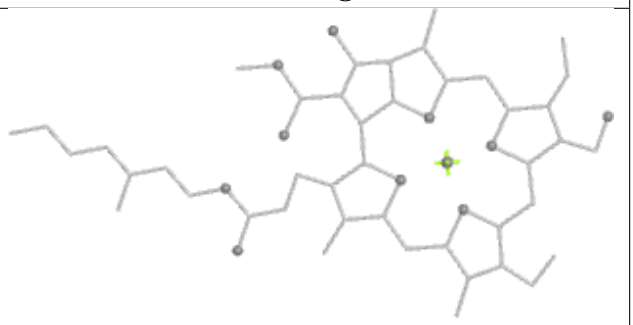
Bond lengths



Bond angles

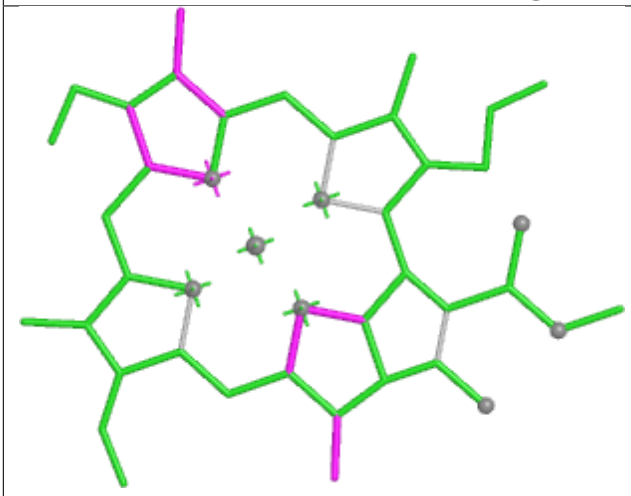


Torsions

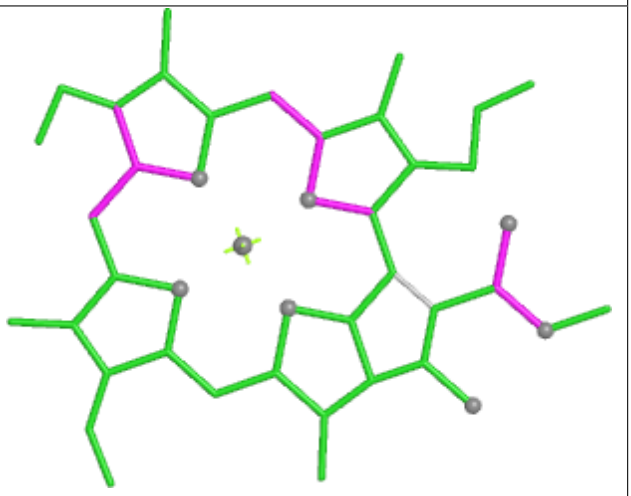


Rings

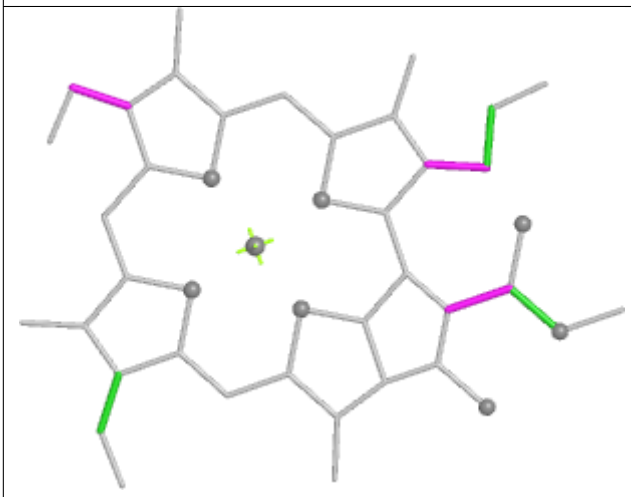
Ligand CLA S 604



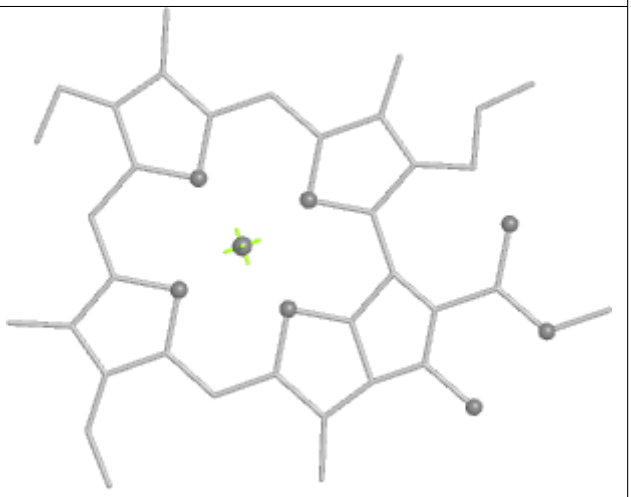
Bond lengths



Bond angles

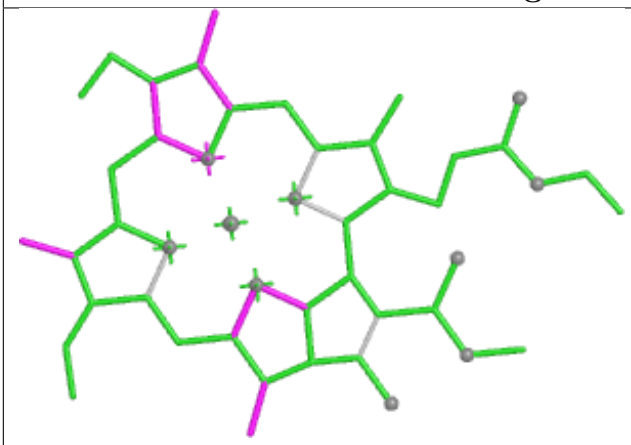


Torsions

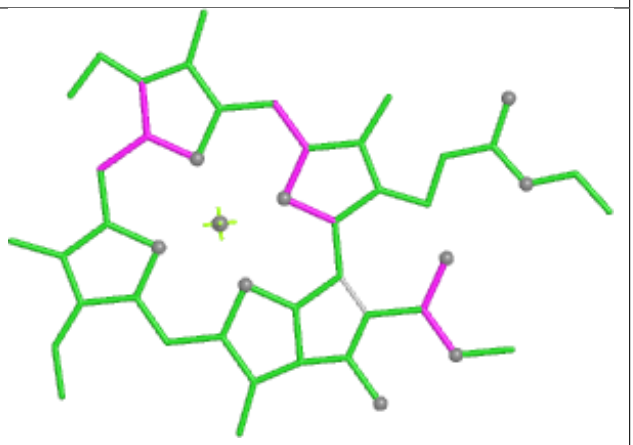


Rings

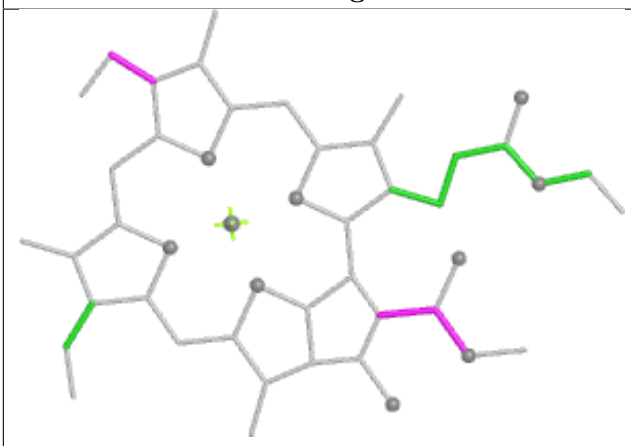
Ligand CLA B 616



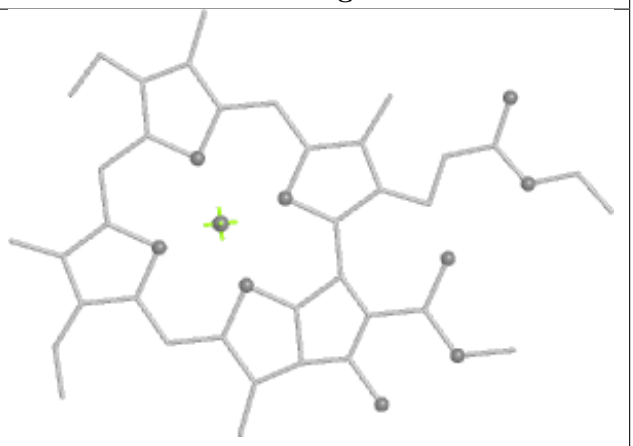
Bond lengths



Bond angles

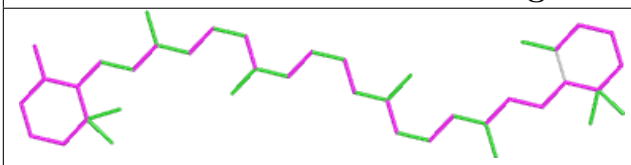


Torsions

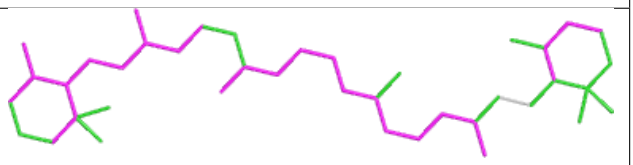


Rings

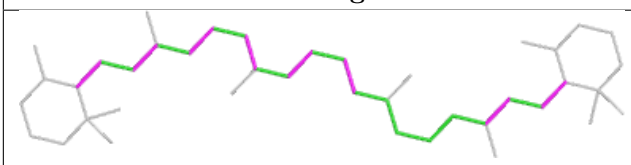
Ligand 8CT T 101



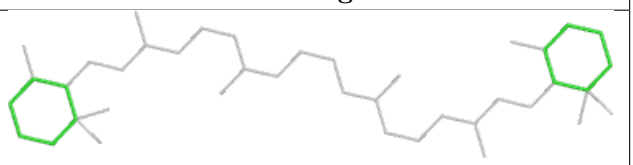
Bond lengths



Bond angles

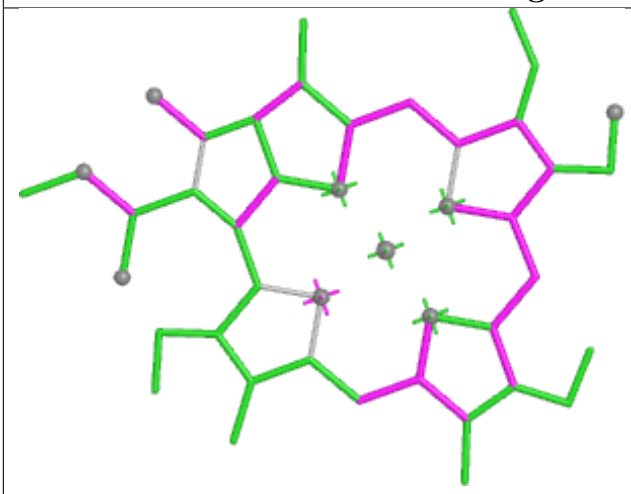


Torsions

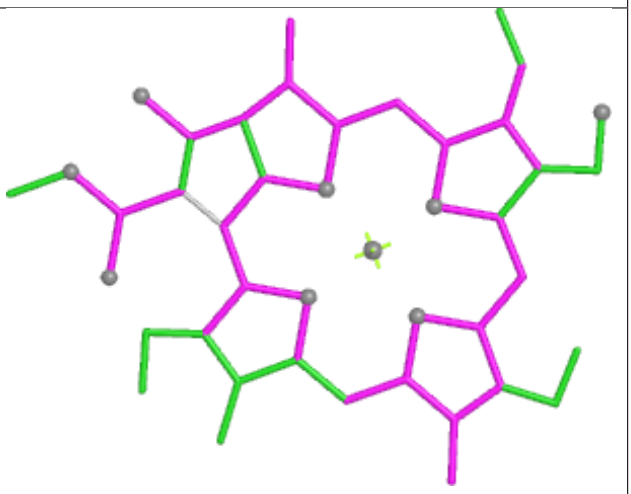


Rings

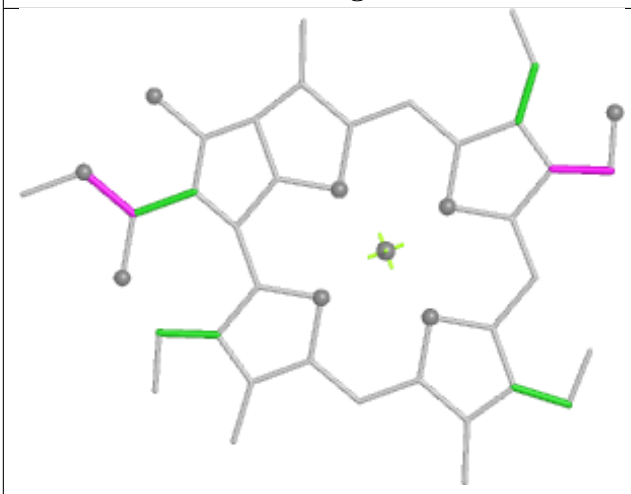
Ligand CHL 1 309



Bond lengths



Bond angles

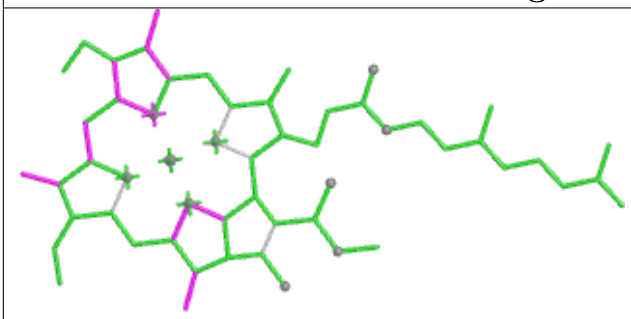


Torsions

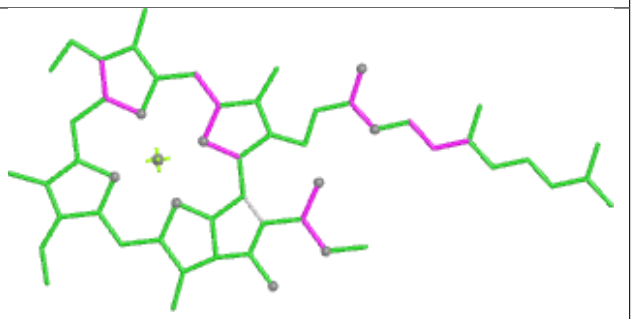


Rings

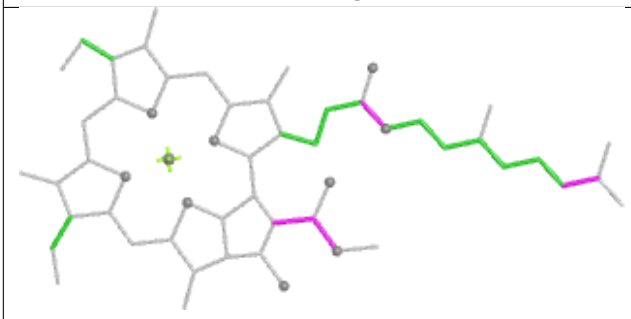
Ligand CLA 7 314



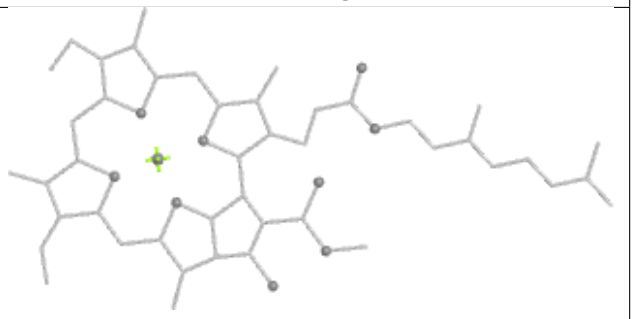
Bond lengths



Bond angles

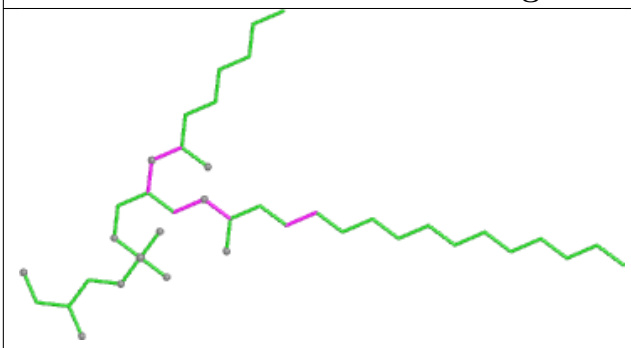


Torsions

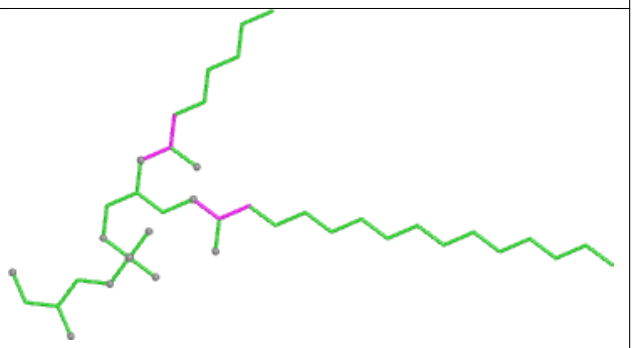


Rings

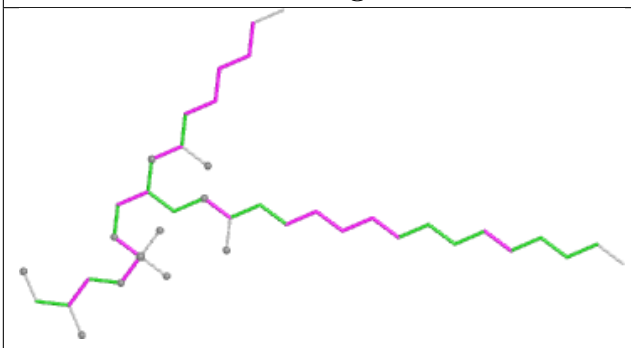
Ligand LHG D 408



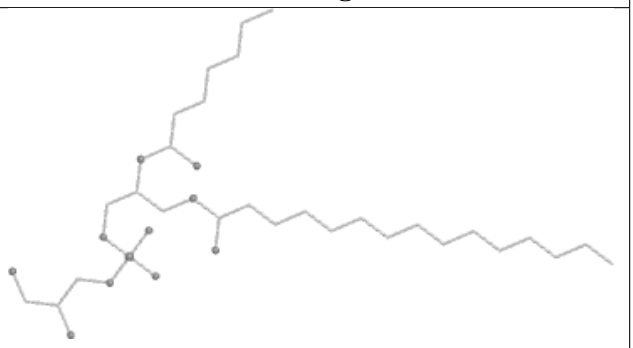
Bond lengths



Bond angles

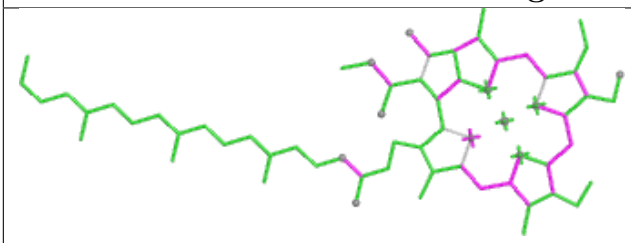


Torsions

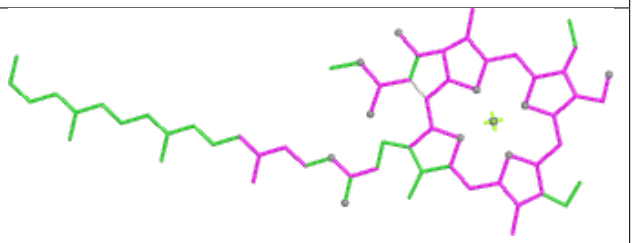


Rings

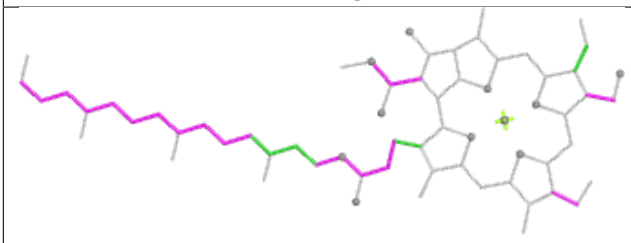
Ligand CHL 7 306



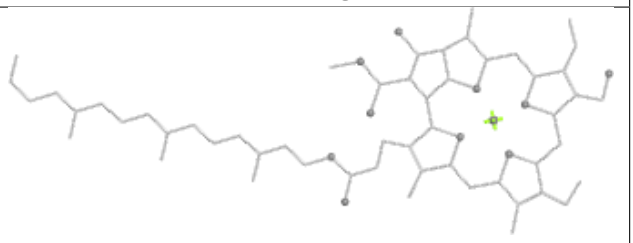
Bond lengths



Bond angles

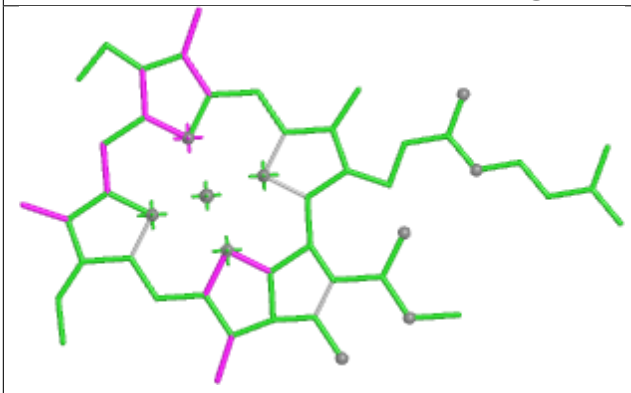


Torsions

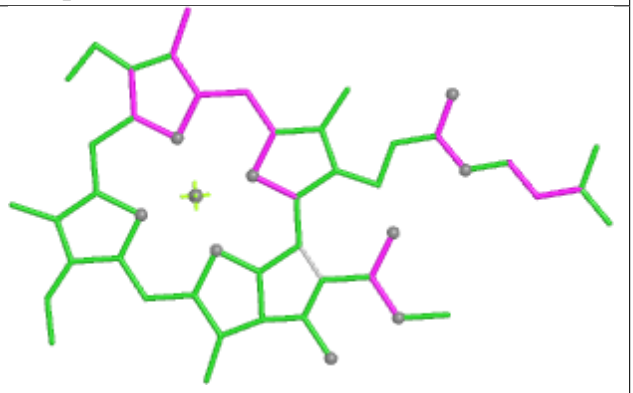


Rings

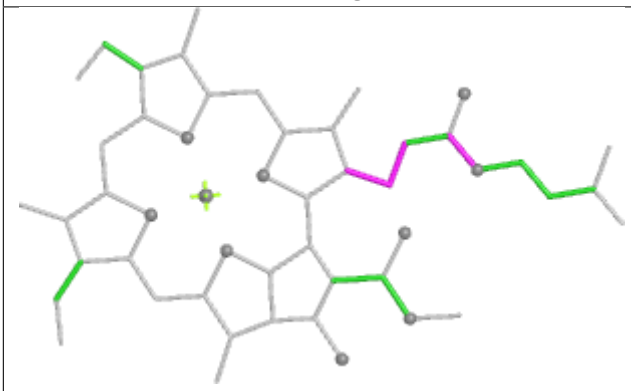
Ligand CLA q 306



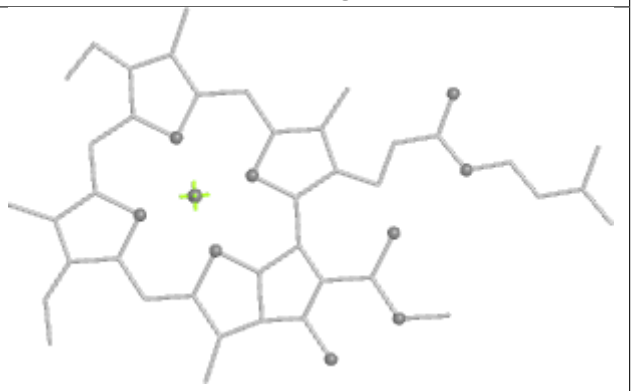
Bond lengths



Bond angles

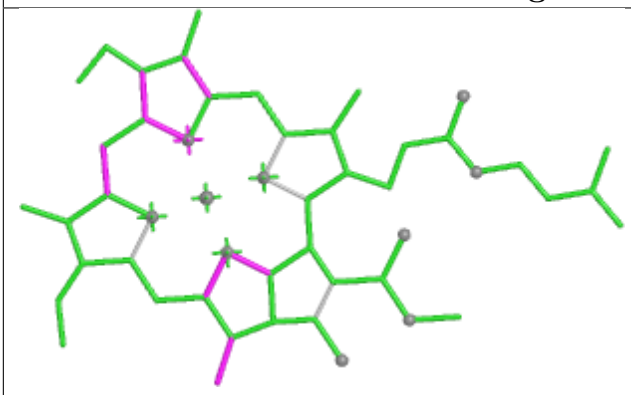


Torsions

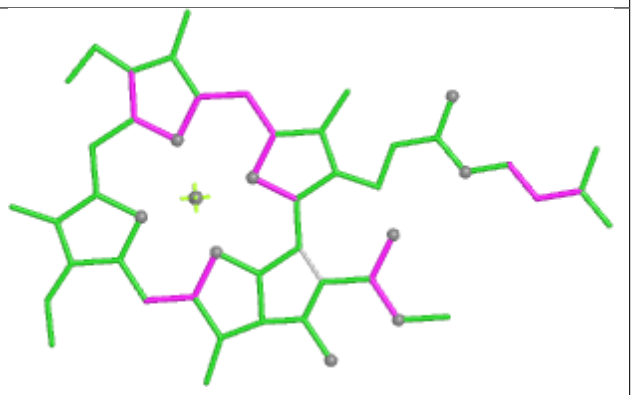


Rings

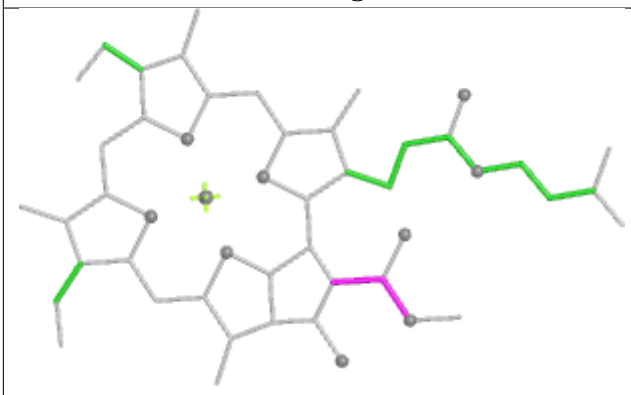
Ligand CLA 2 308



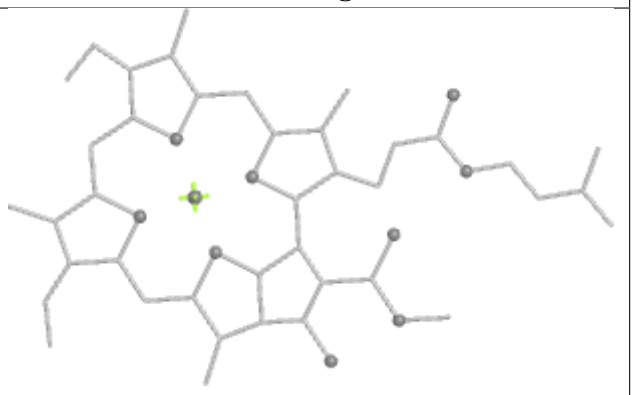
Bond lengths



Bond angles

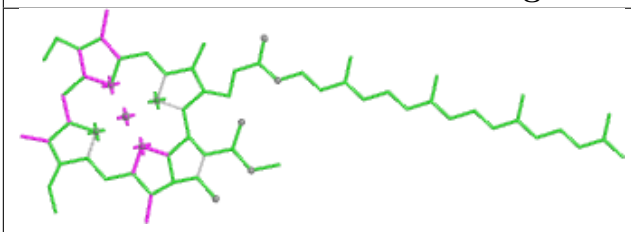


Torsions

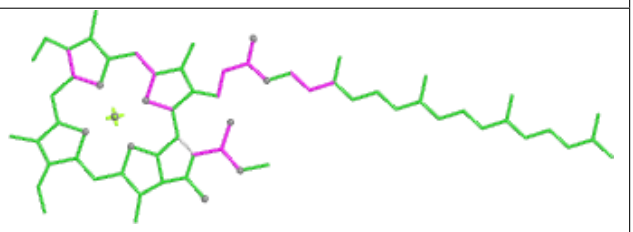


Rings

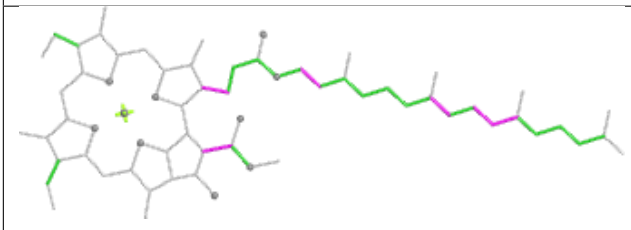
Ligand CLA D 404



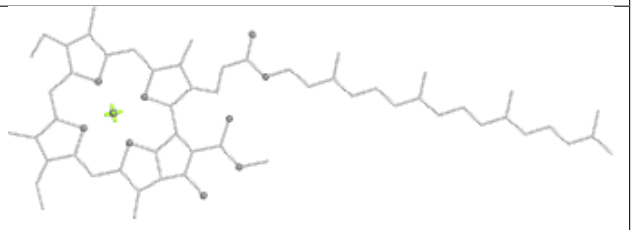
Bond lengths



Bond angles

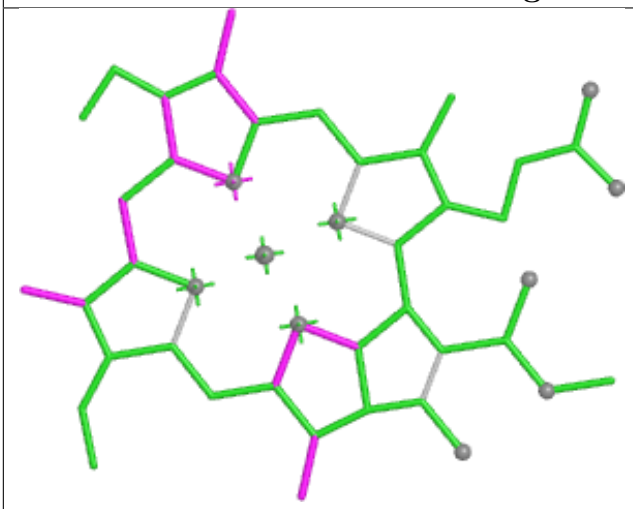


Torsions

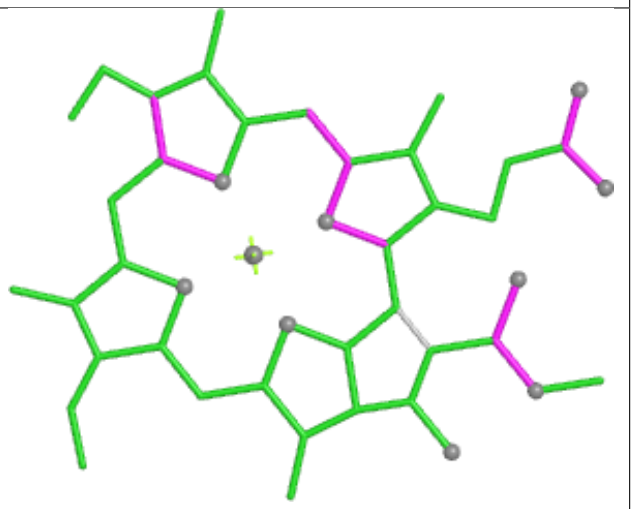


Rings

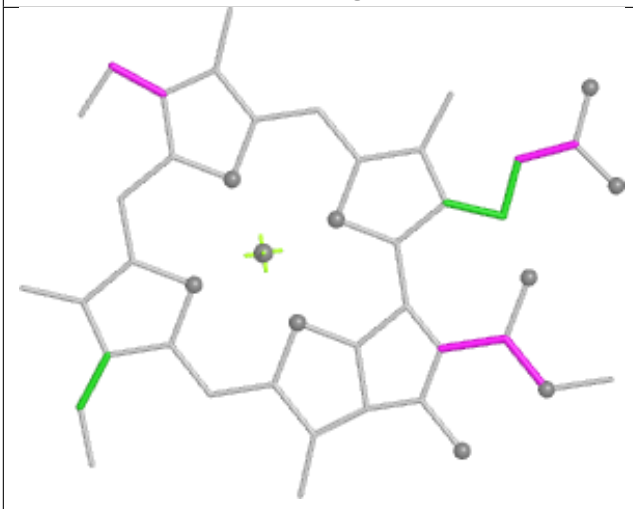
Ligand CLA N 315



Bond lengths



Bond angles

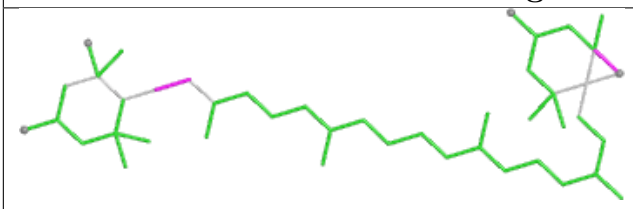


Torsions

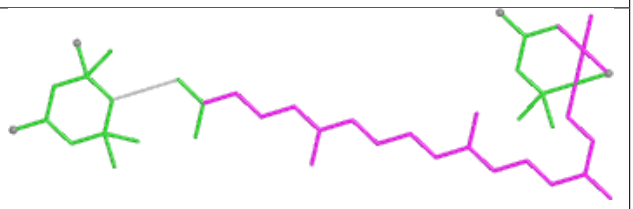


Rings

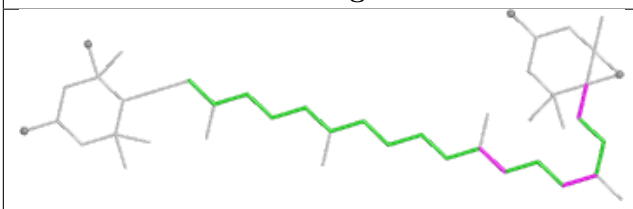
Ligand NEX 2 304



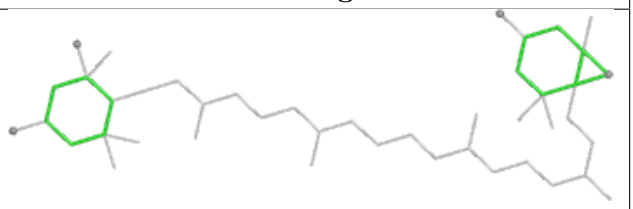
Bond lengths



Bond angles

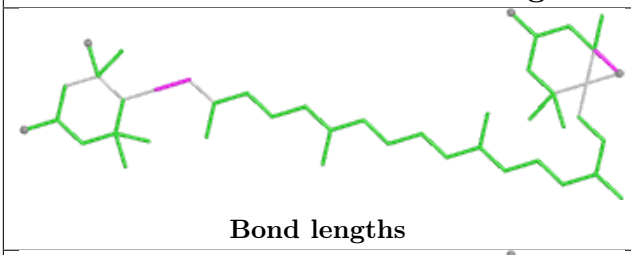


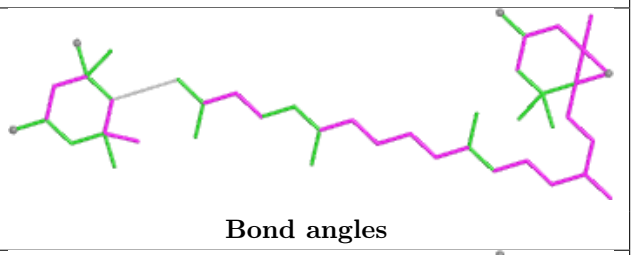
Torsions

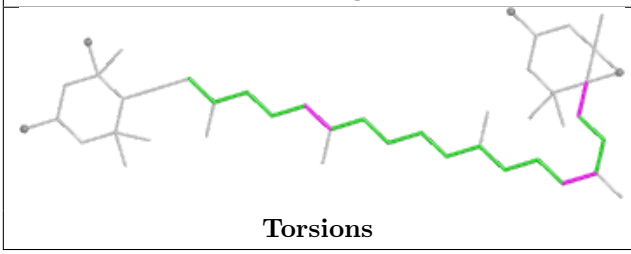


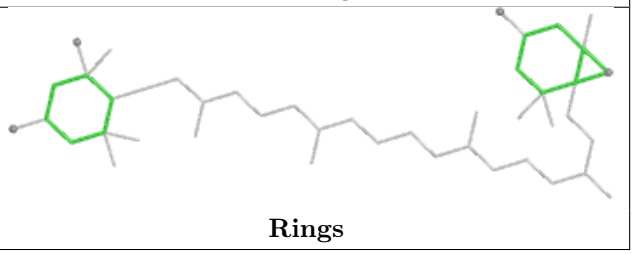
Rings

Ligand NEX r 301

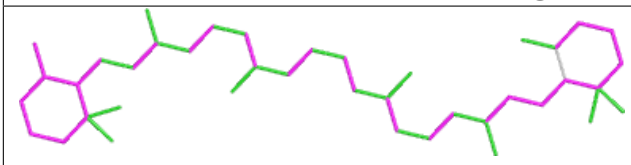

Bond lengths

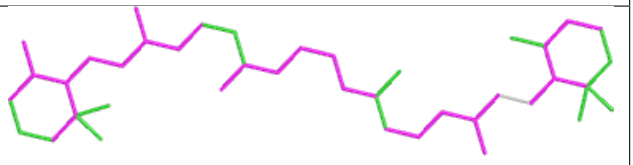

Bond angles

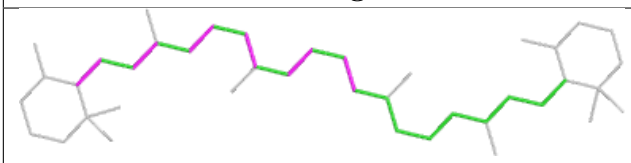

Torsions

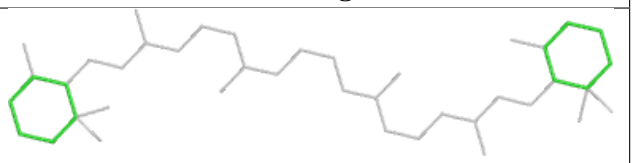

Rings

Ligand 8CT a 608

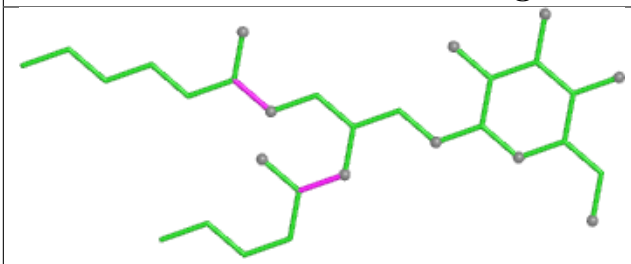

Bond lengths

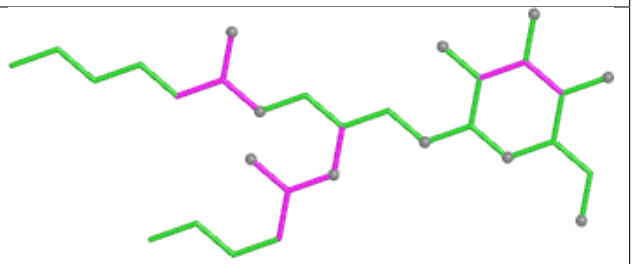

Bond angles

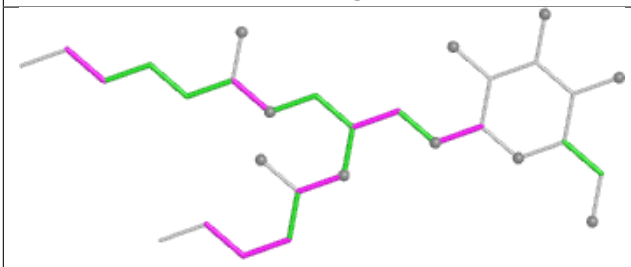

Torsions

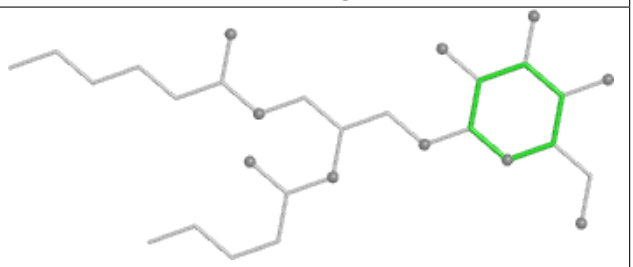

Rings

Ligand LMG W 201

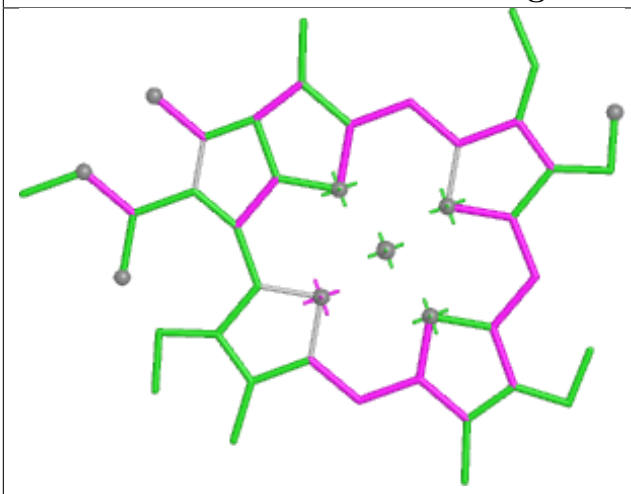

Bond lengths


Bond angles

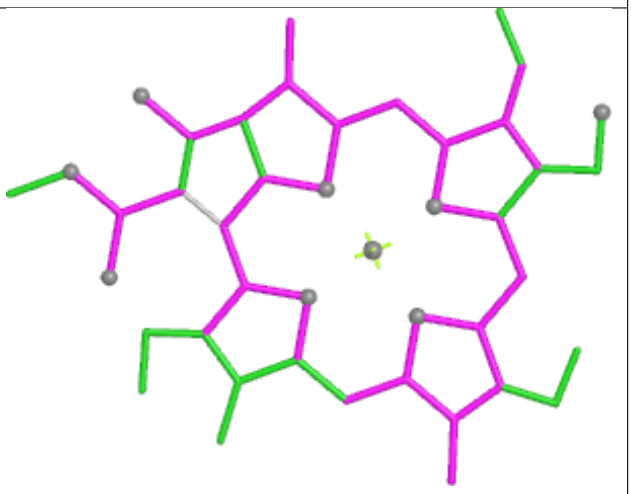

Torsions


Rings

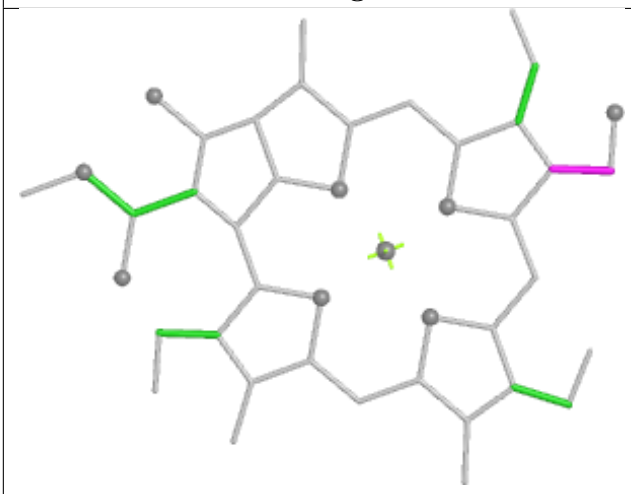
Ligand CHL 8 307



Bond lengths



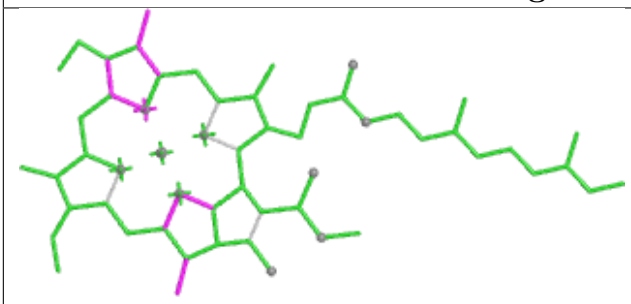
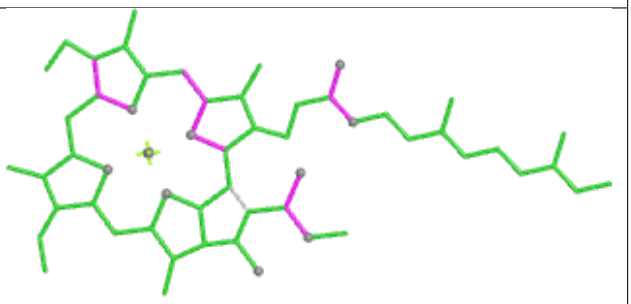
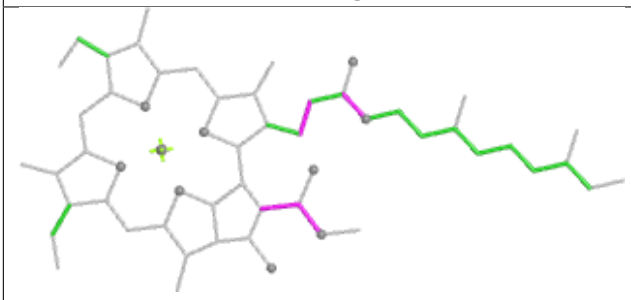
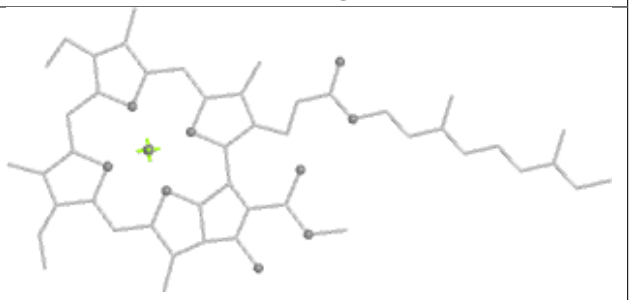
Bond angles

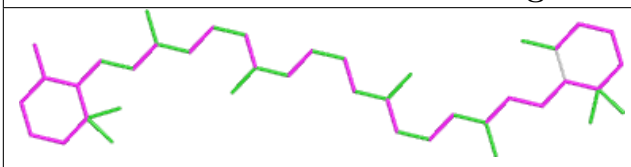
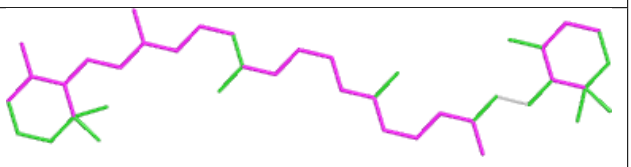
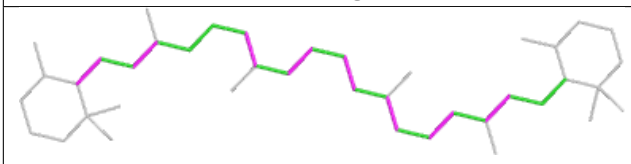
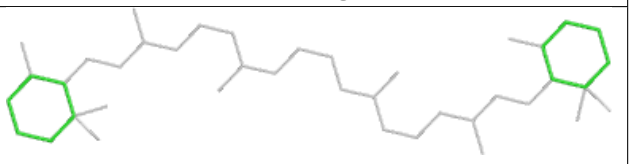


Torsions

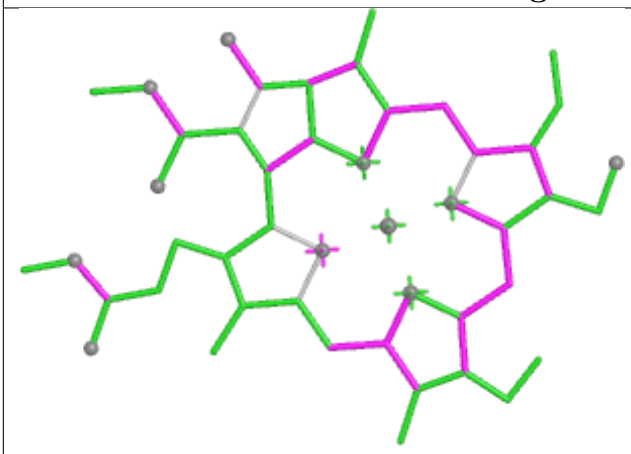


Rings

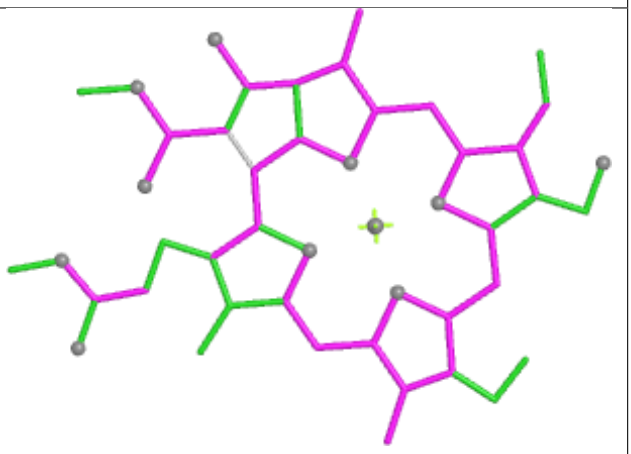
Ligand CLA 7 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT C 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

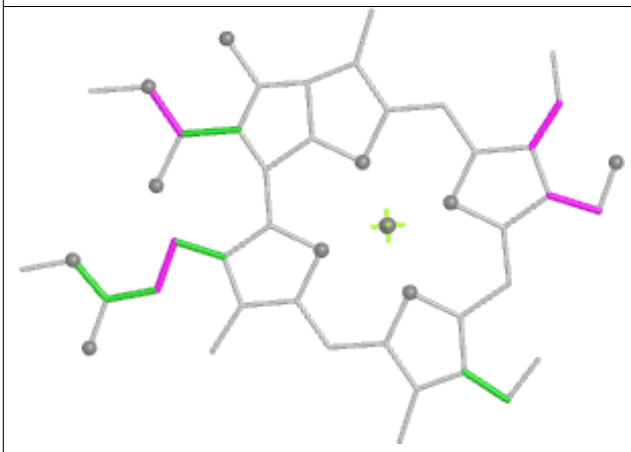
Ligand CHL s 409



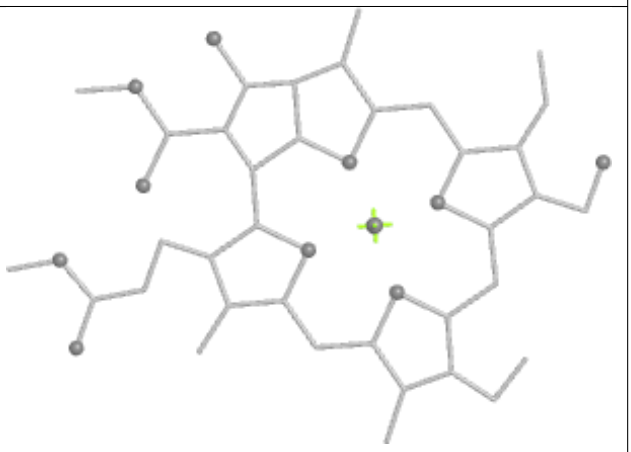
Bond lengths



Bond angles

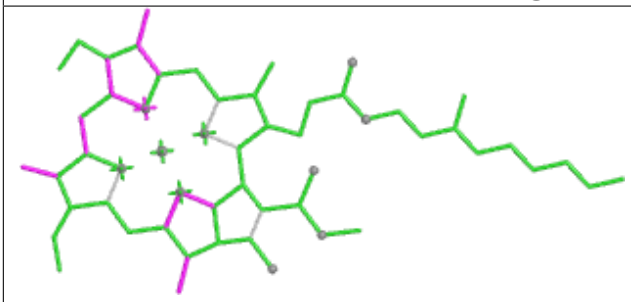


Torsions

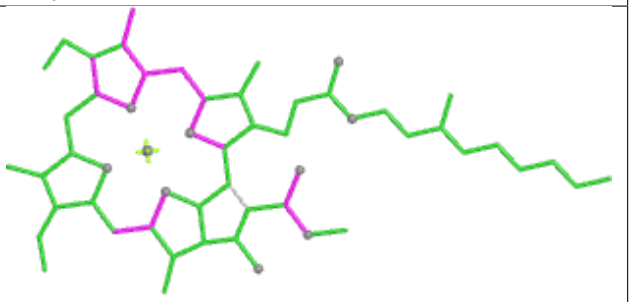


Rings

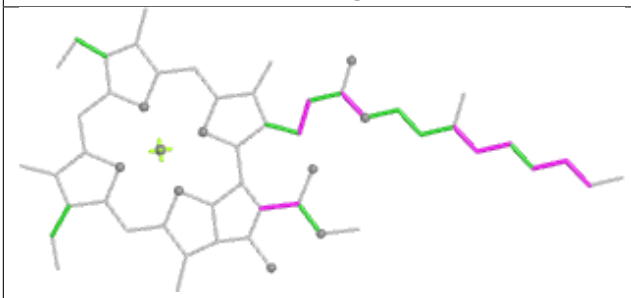
Ligand CLA y 317



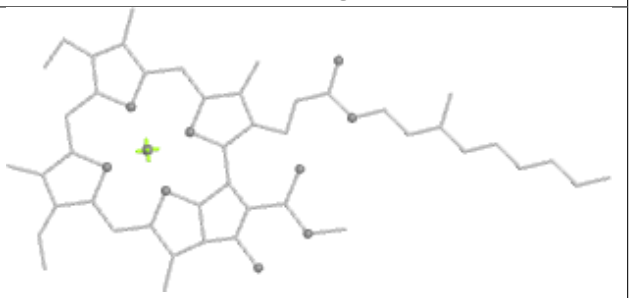
Bond lengths



Bond angles

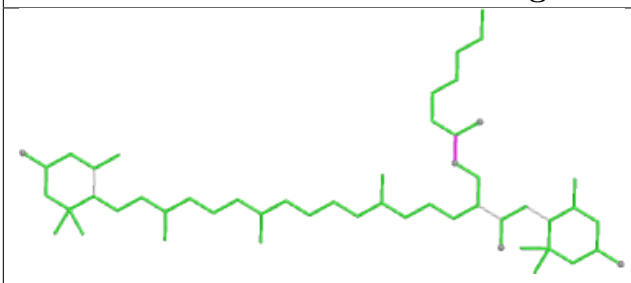


Torsions

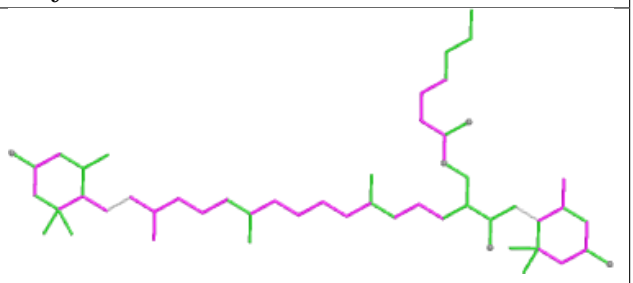


Rings

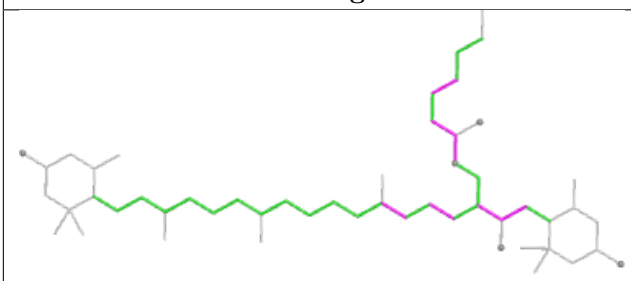
Ligand 0UR y 301



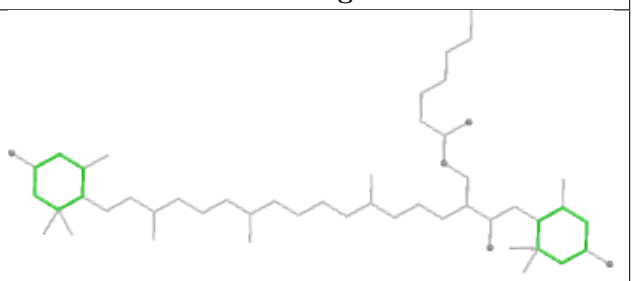
Bond lengths



Bond angles

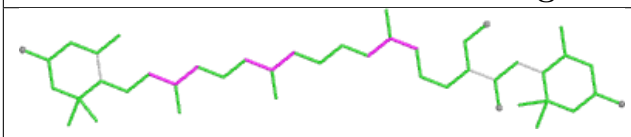


Torsions

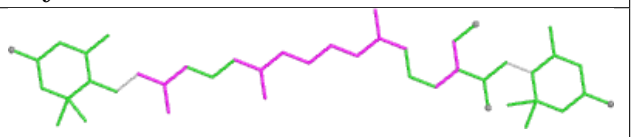


Rings

Ligand 0IE y 303



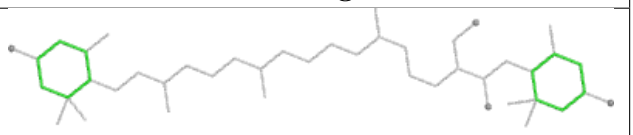
Bond lengths



Bond angles

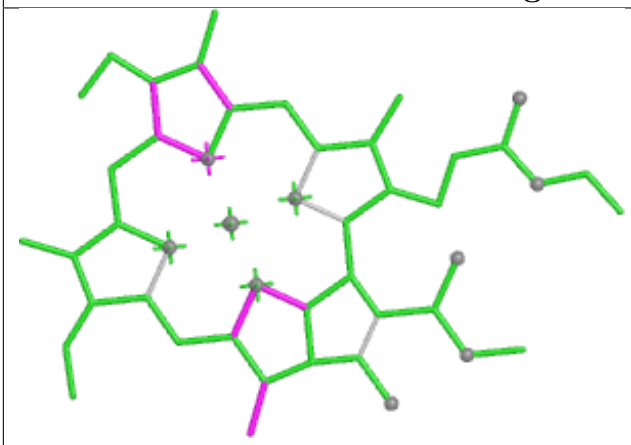


Torsions

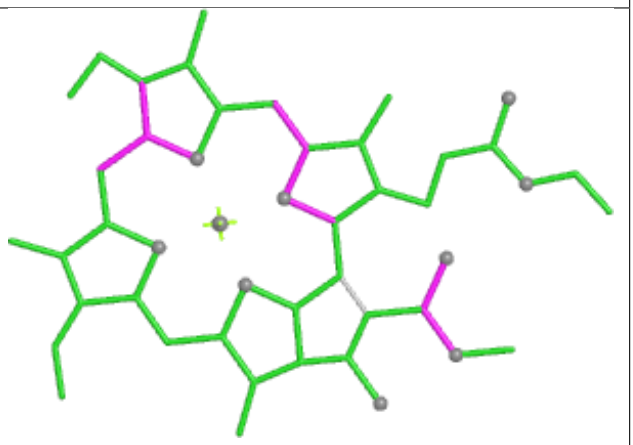


Rings

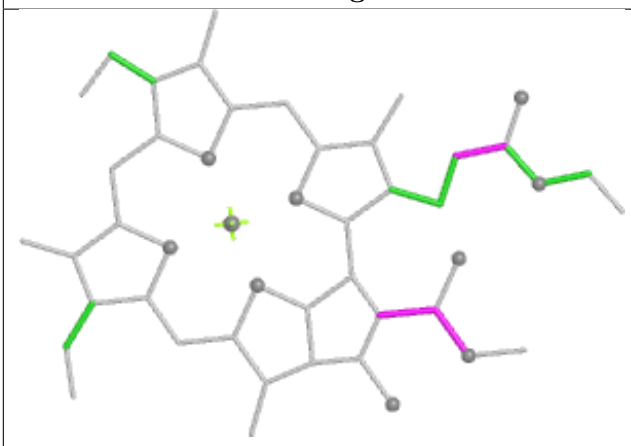
Ligand CLA R 603



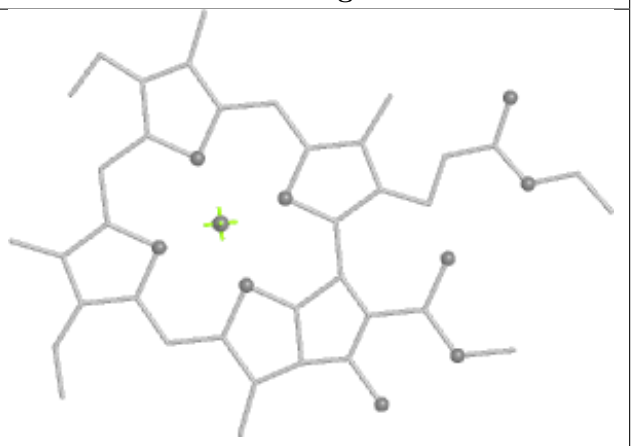
Bond lengths



Bond angles

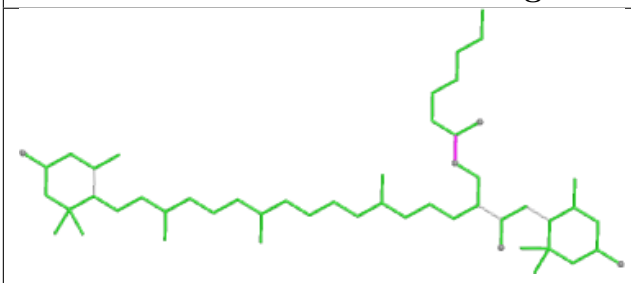


Torsions

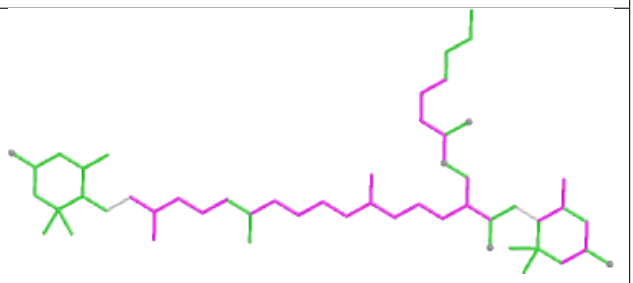


Rings

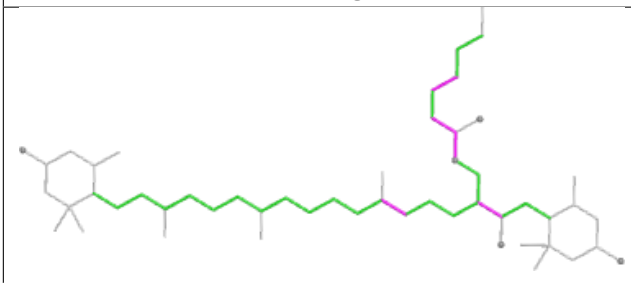
Ligand 0UR G 301



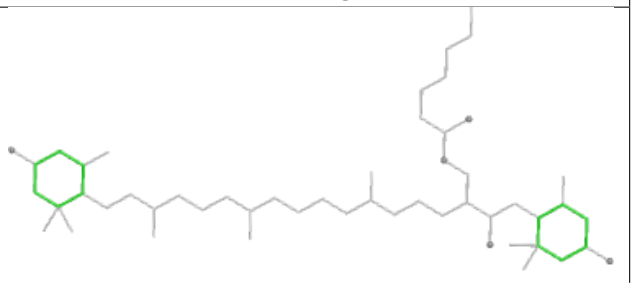
Bond lengths



Bond angles

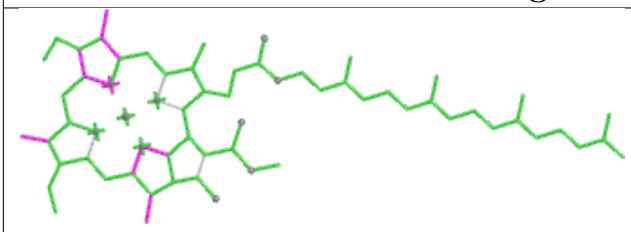


Torsions

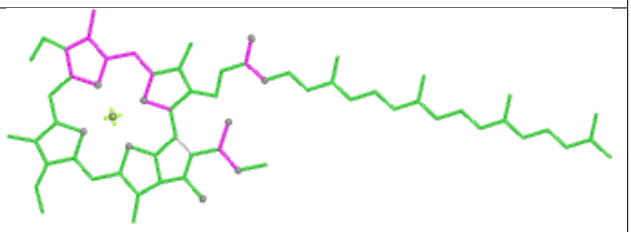


Rings

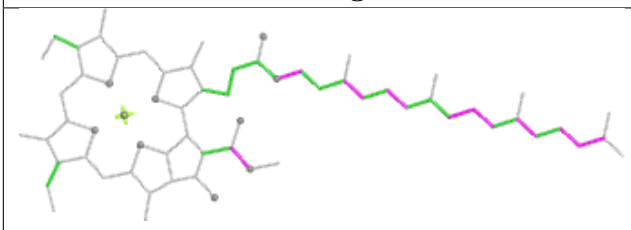
Ligand CLA c 603



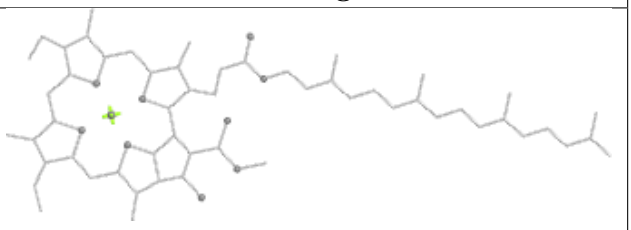
Bond lengths



Bond angles

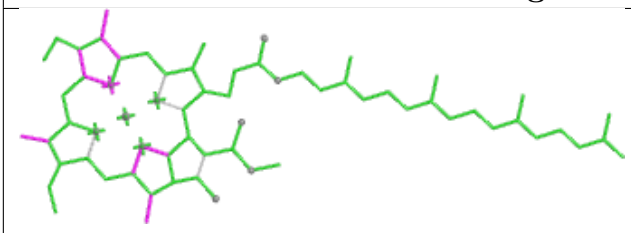


Torsions

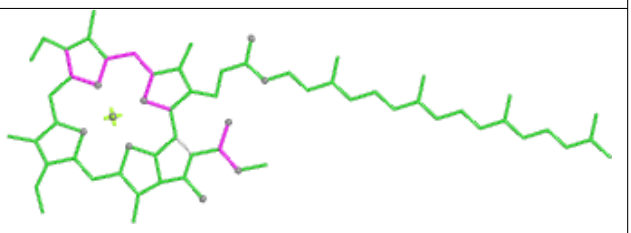


Rings

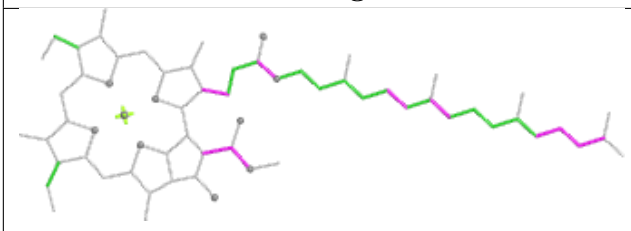
Ligand CLA d 405



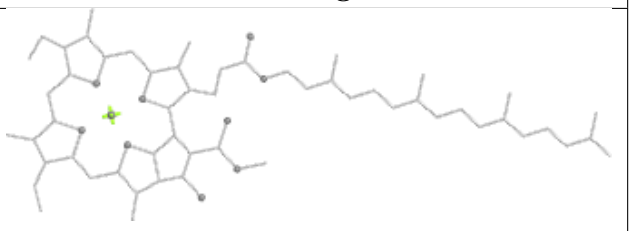
Bond lengths



Bond angles

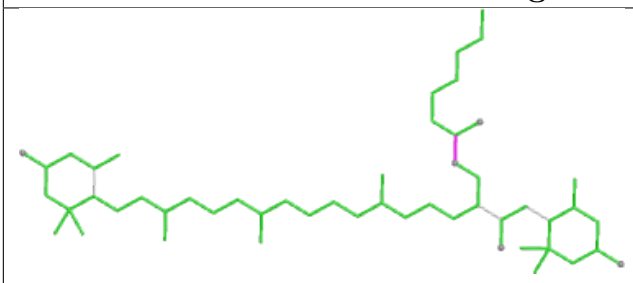


Torsions

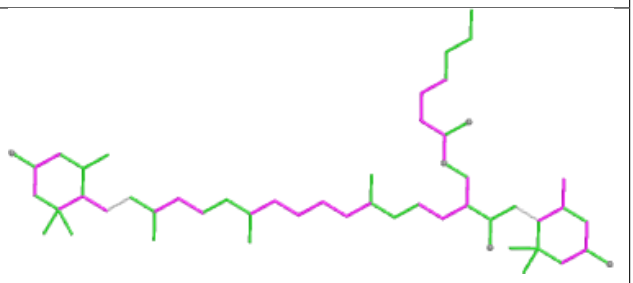


Rings

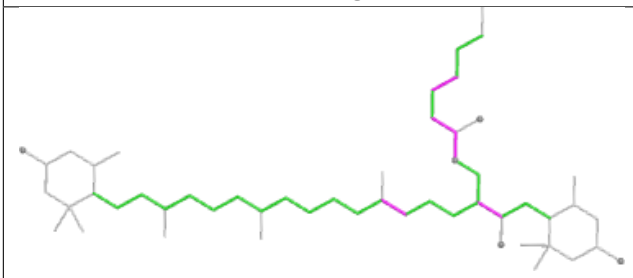
Ligand 0UR n 301



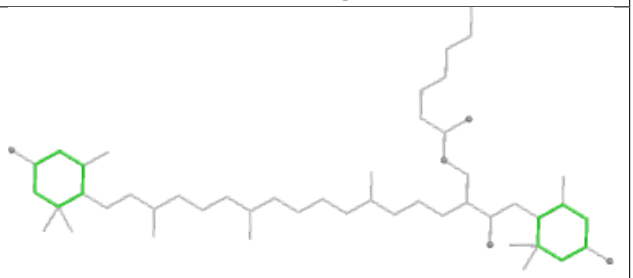
Bond lengths



Bond angles

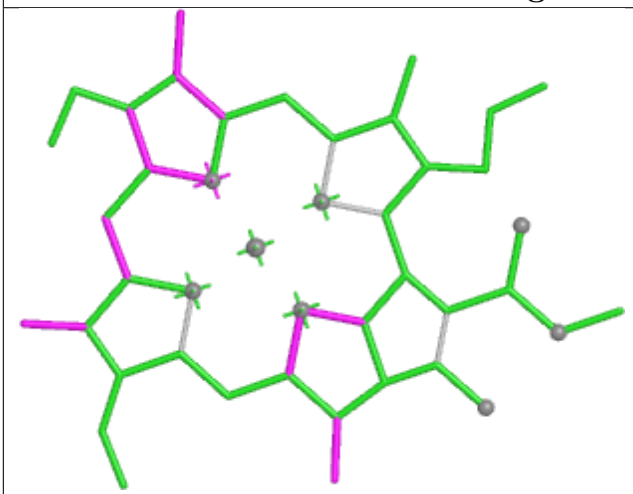


Torsions

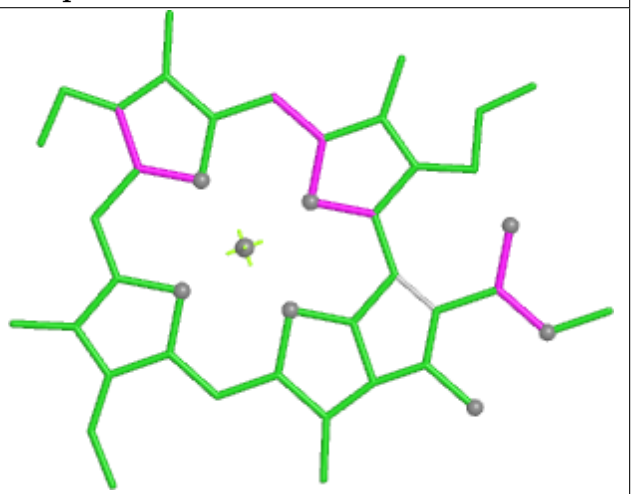


Rings

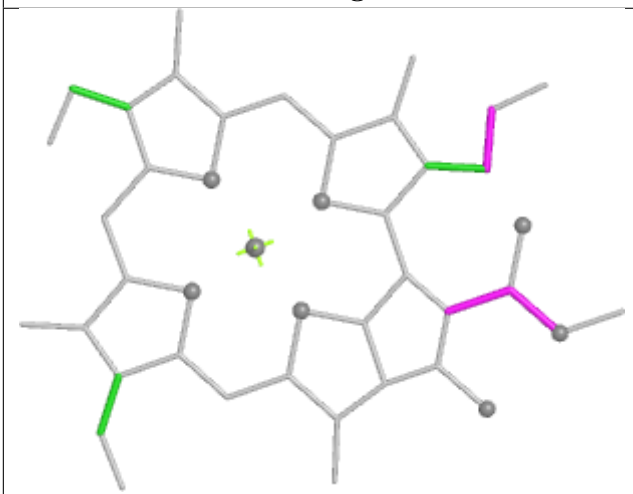
Ligand CLA q 315



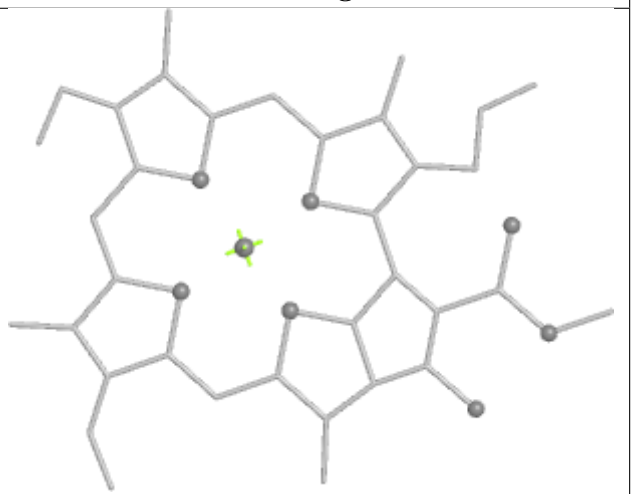
Bond lengths



Bond angles

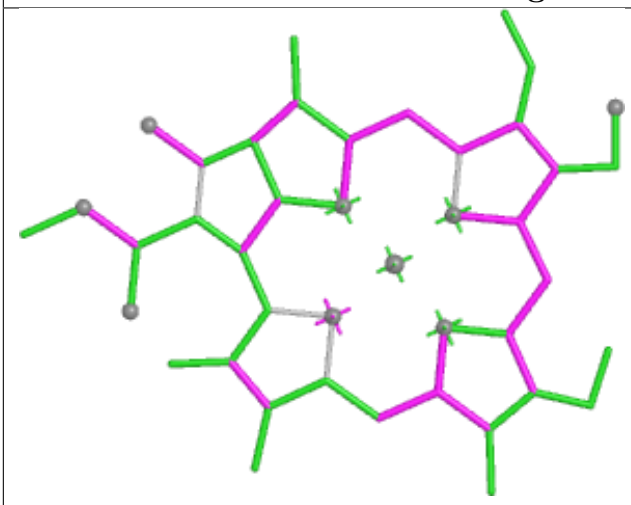


Torsions

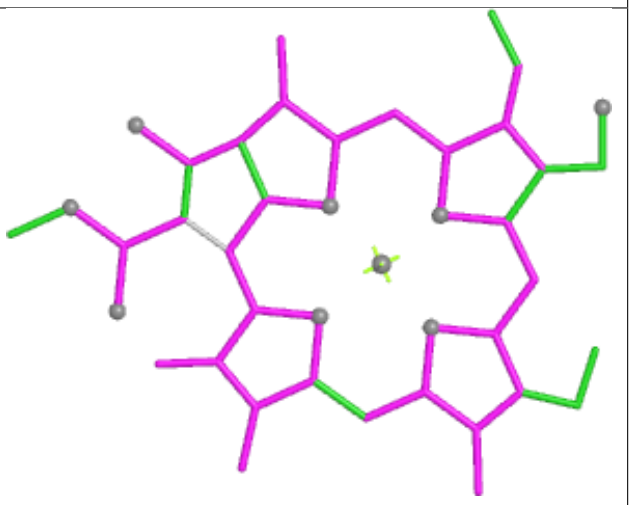


Rings

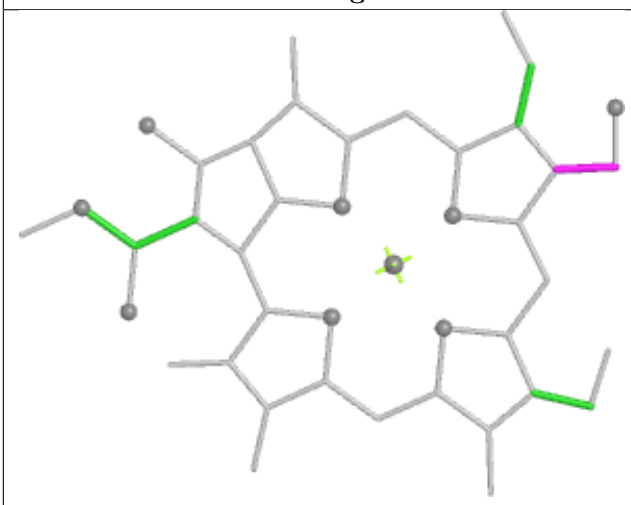
Ligand CHL 3 317



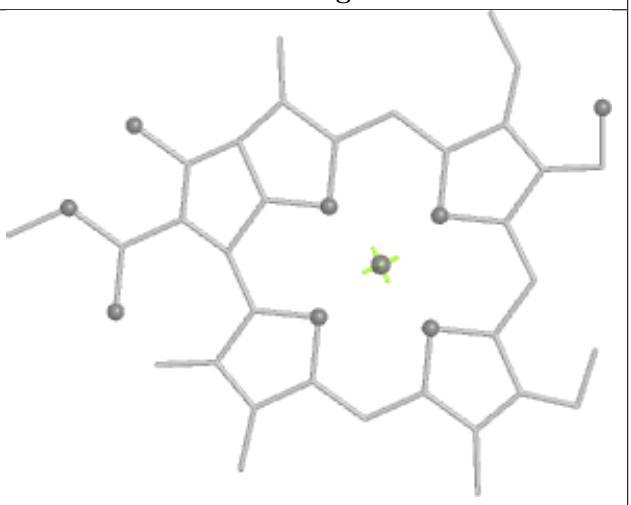
Bond lengths



Bond angles

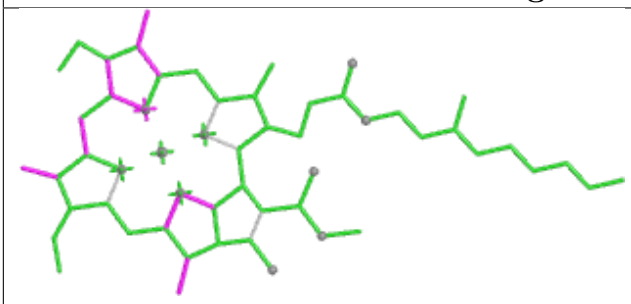


Torsions

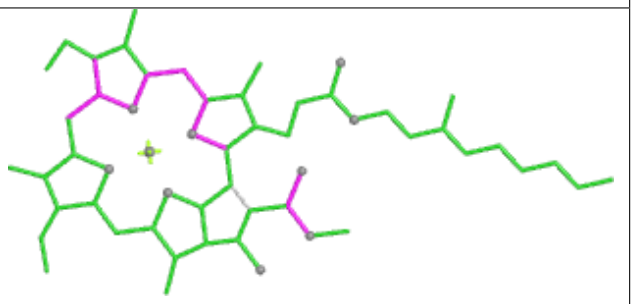


Rings

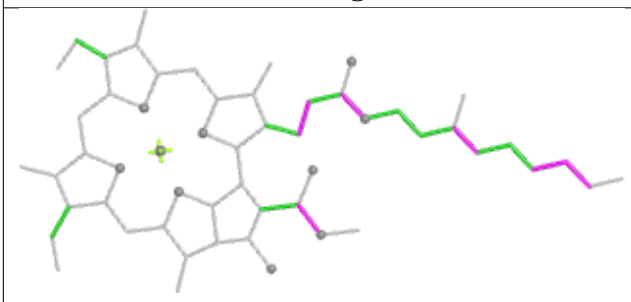
Ligand CLA S 612



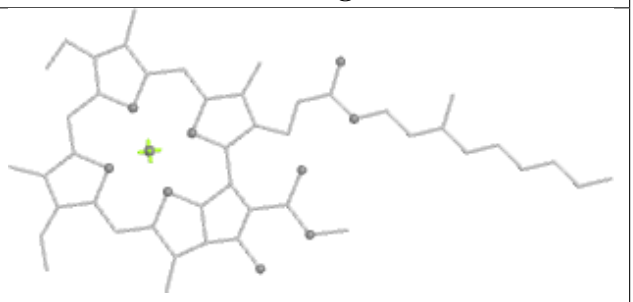
Bond lengths



Bond angles

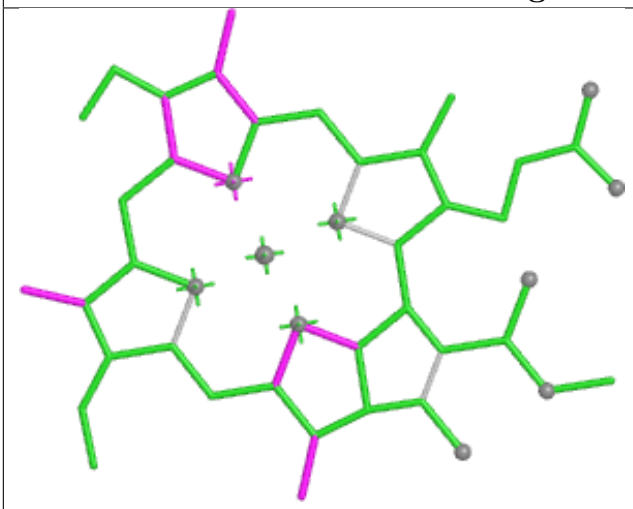


Torsions

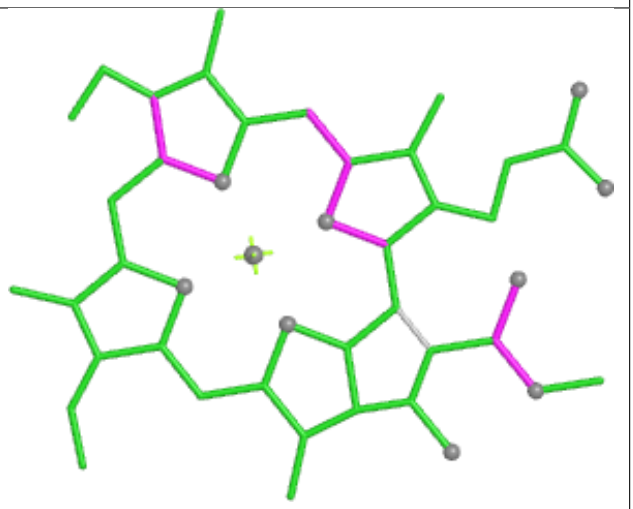


Rings

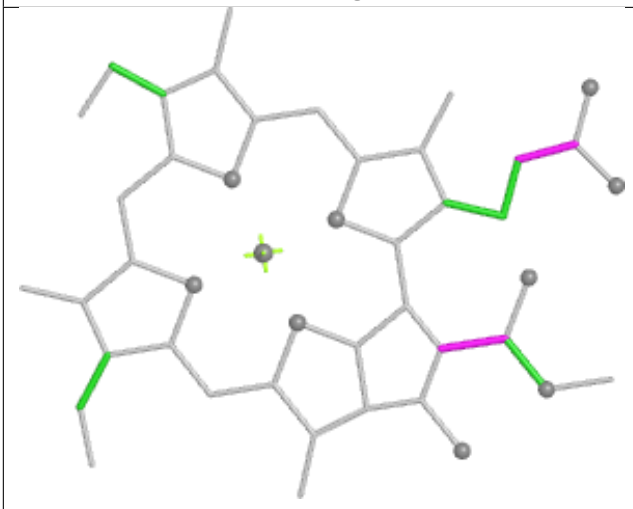
Ligand CLA 8 313



Bond lengths



Bond angles

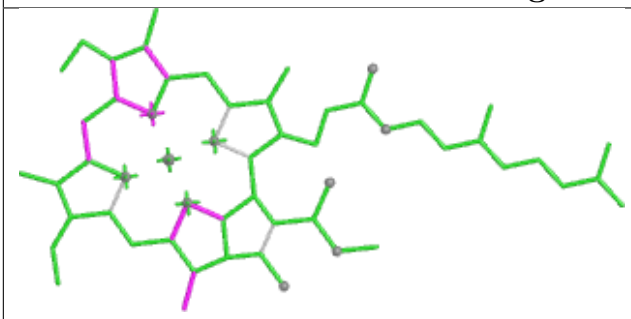


Torsions

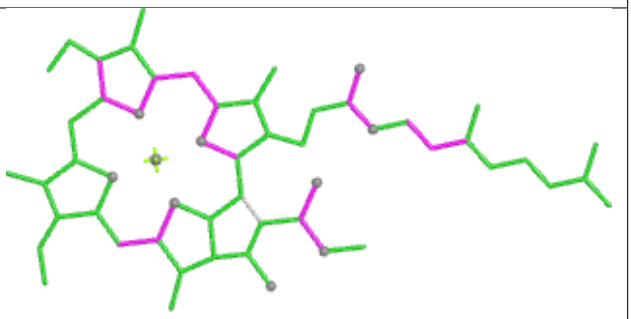


Rings

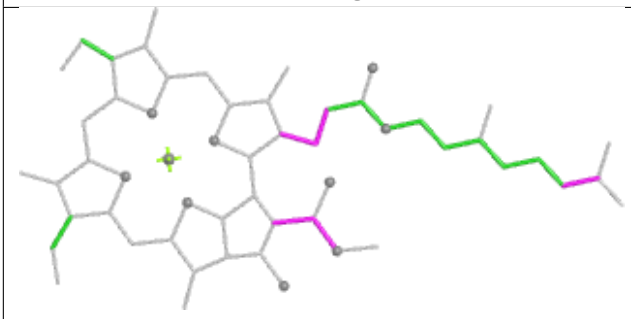
Ligand CLA 4 313



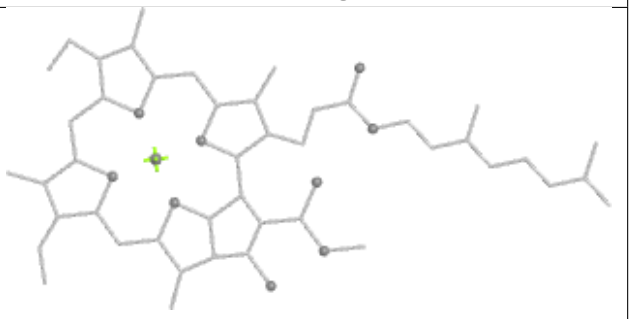
Bond lengths



Bond angles

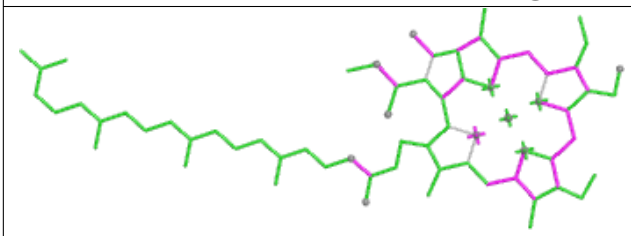


Torsions

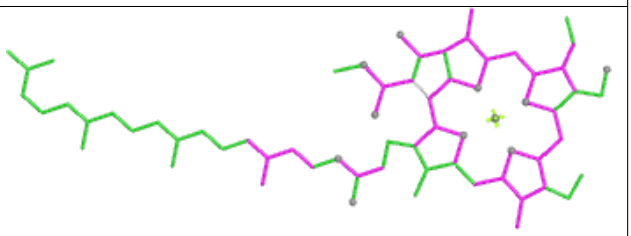


Rings

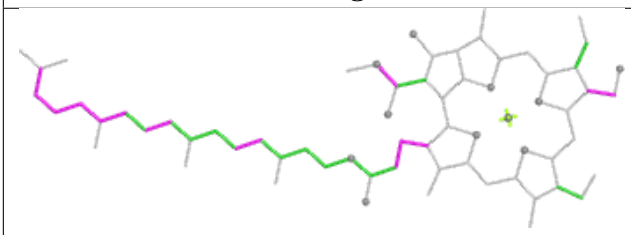
Ligand CHL u 305



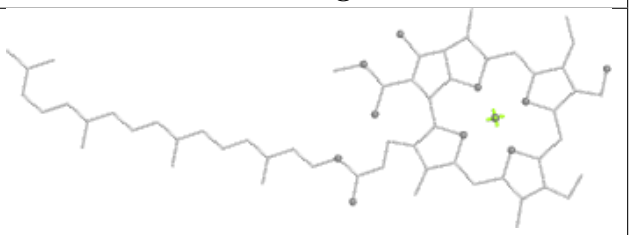
Bond lengths



Bond angles

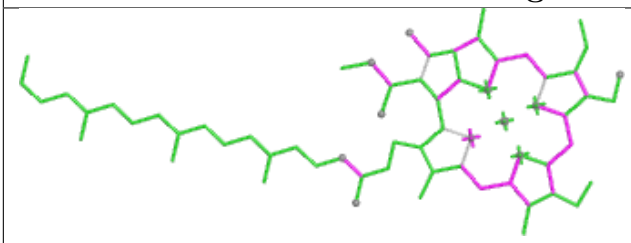


Torsions

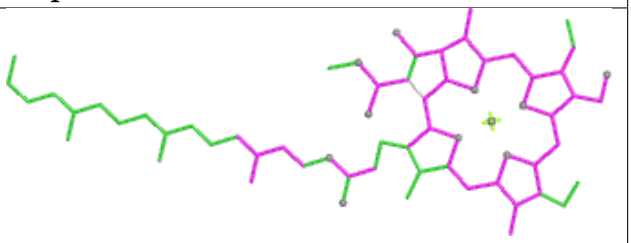


Rings

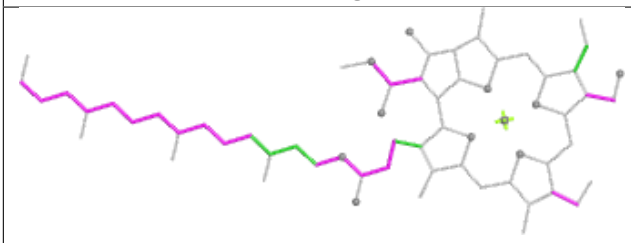
Ligand CHL p 306



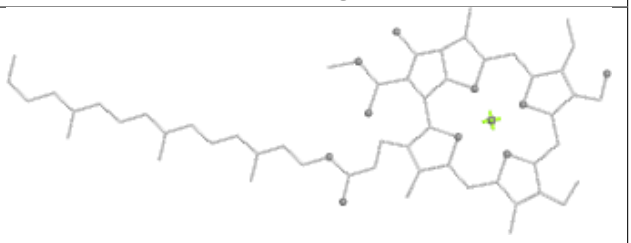
Bond lengths



Bond angles

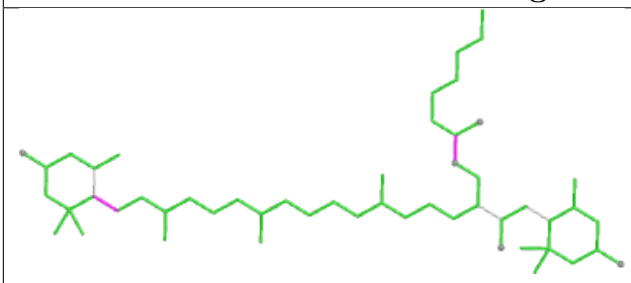


Torsions

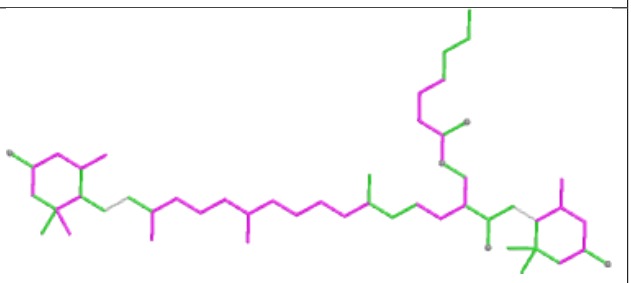


Rings

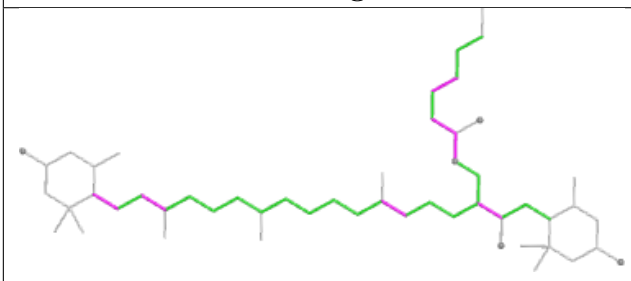
Ligand 0UR 4 301



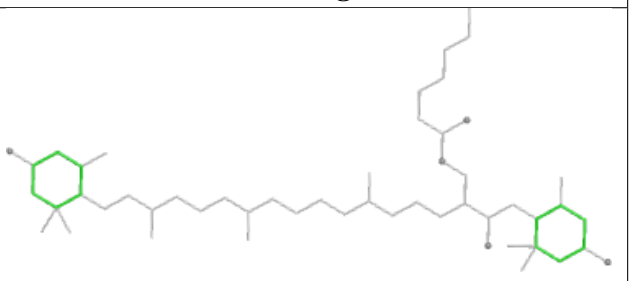
Bond lengths



Bond angles

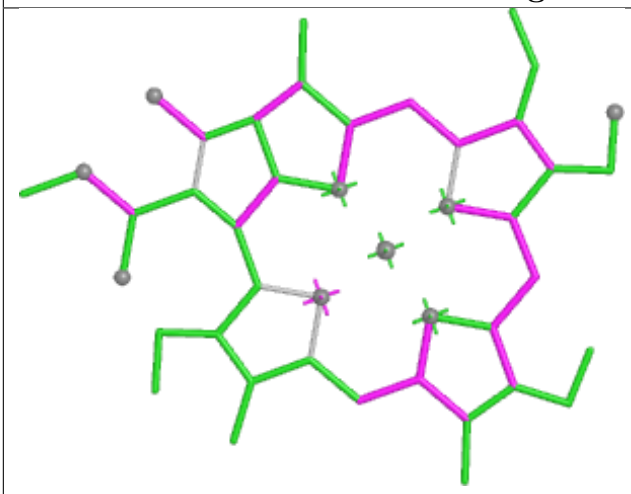


Torsions

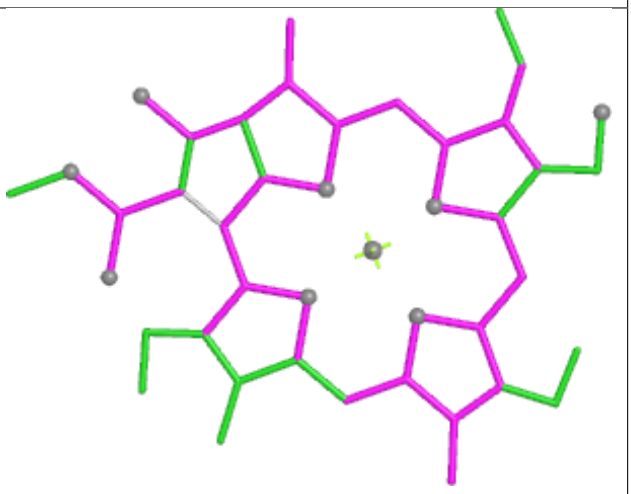


Rings

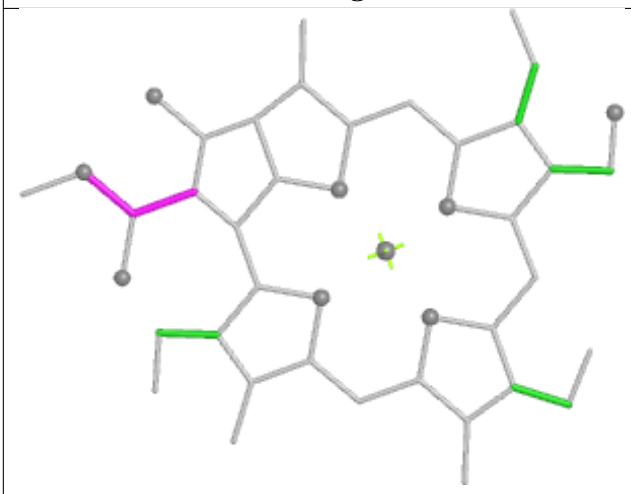
Ligand CHL 5 309



Bond lengths



Bond angles

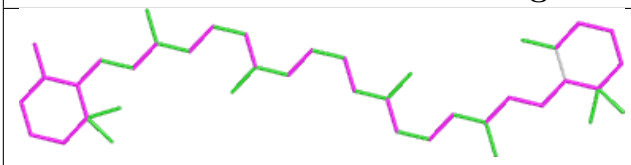


Torsions

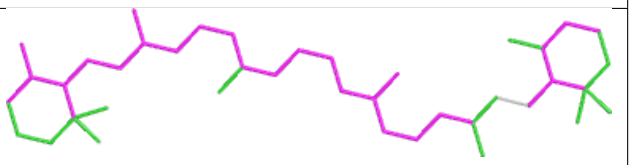


Rings

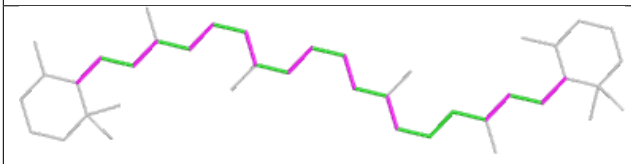
Ligand 8CT b 617



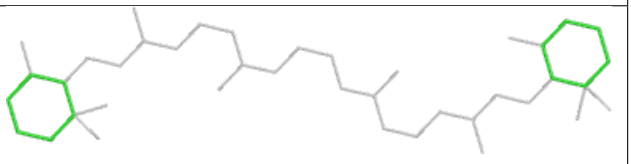
Bond lengths



Bond angles

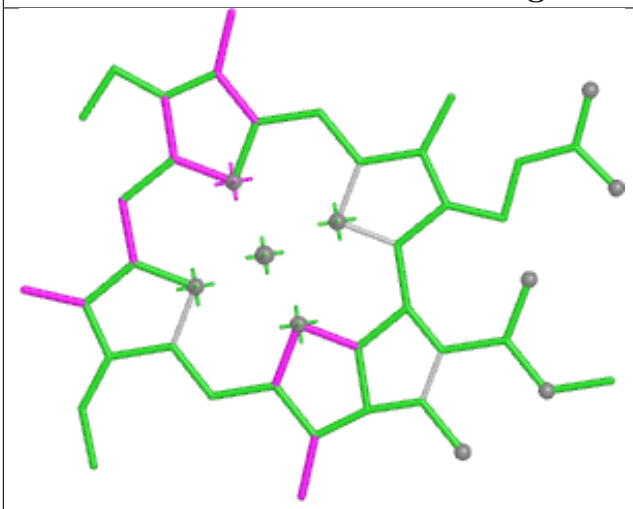


Torsions

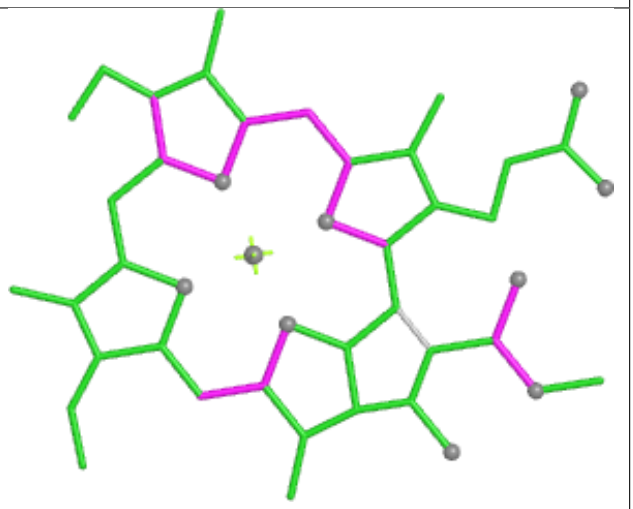


Rings

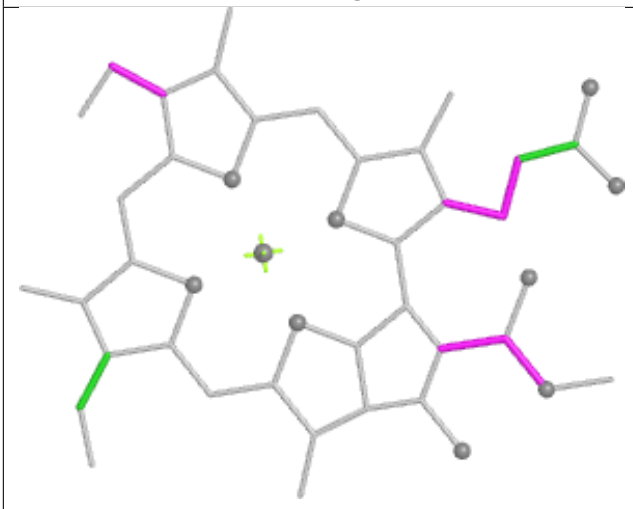
Ligand CLA b 601



Bond lengths



Bond angles

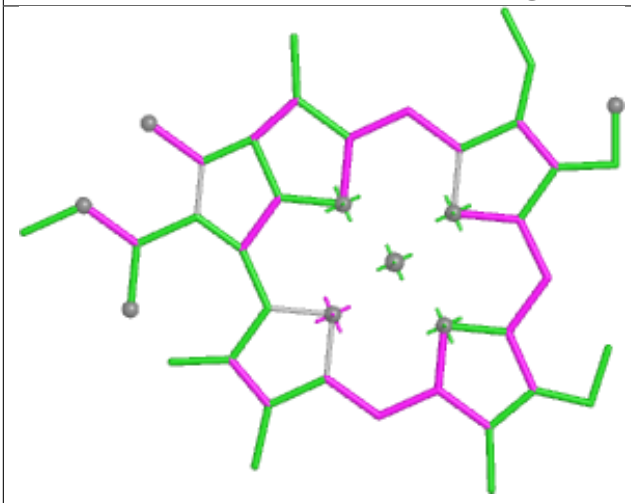


Torsions

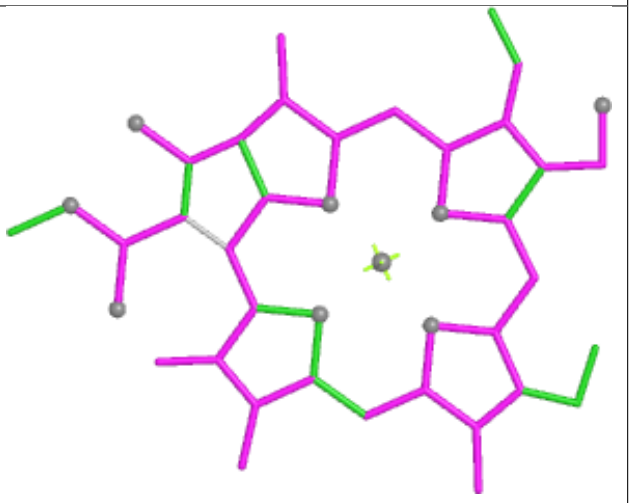


Rings

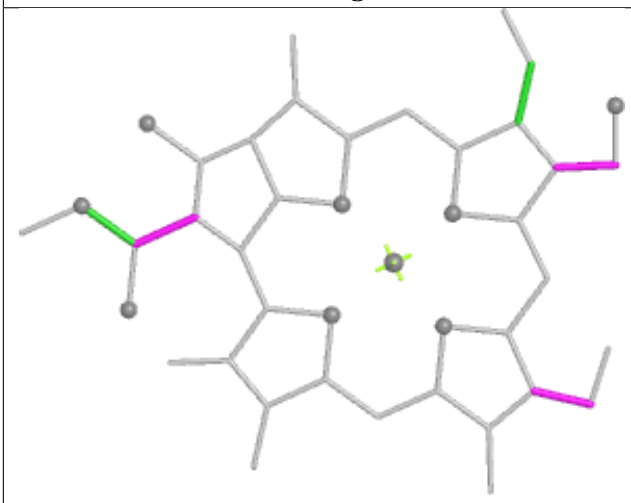
Ligand CHL Y 317



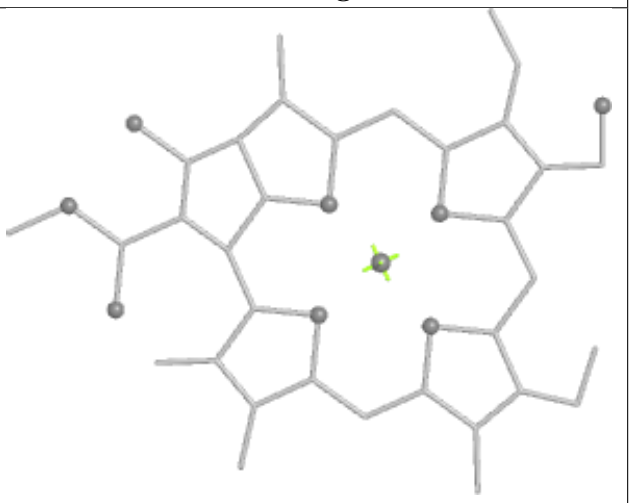
Bond lengths



Bond angles

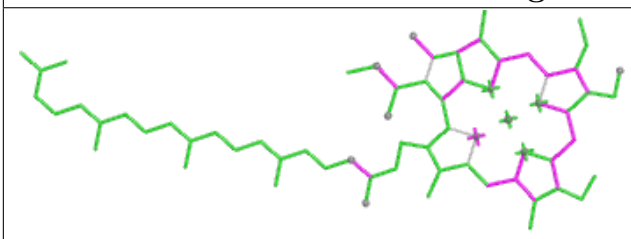


Torsions

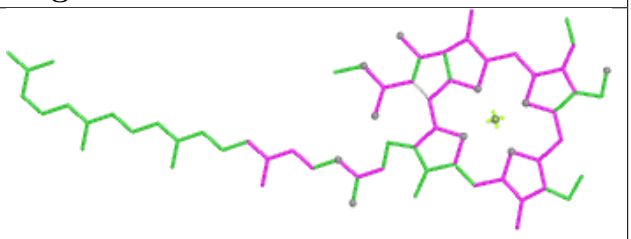


Rings

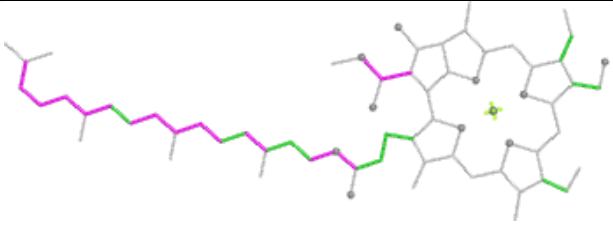
Ligand CHL g 313



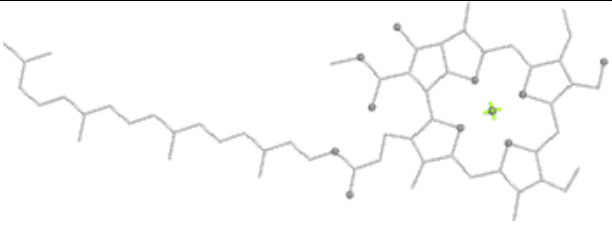
Bond lengths



Bond angles

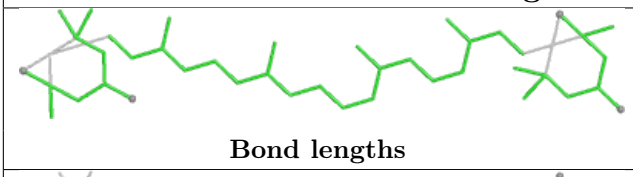


Torsions

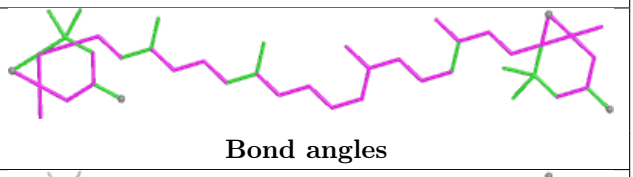


Rings

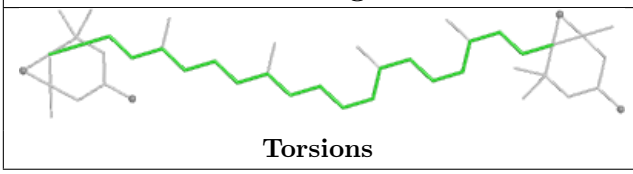
Ligand XAT R 615



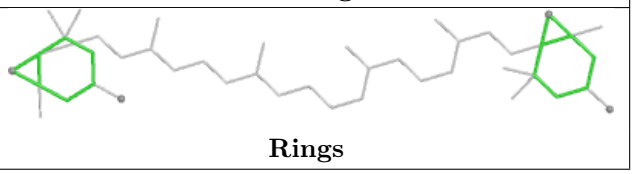
Bond lengths



Bond angles

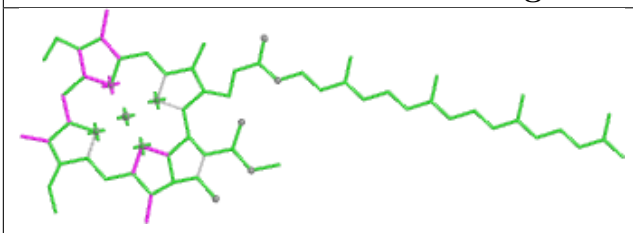


Torsions

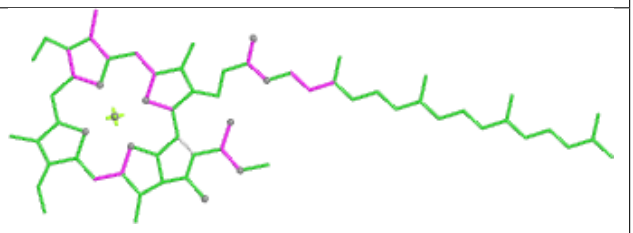


Rings

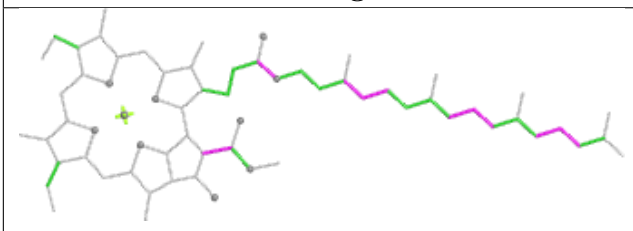
Ligand CLA C 610



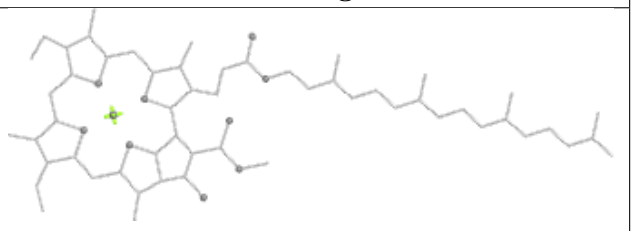
Bond lengths



Bond angles

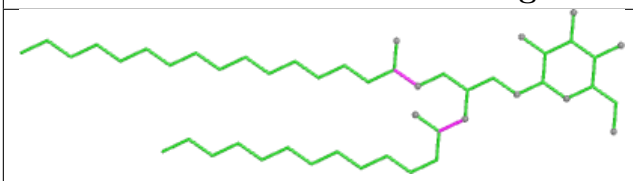


Torsions

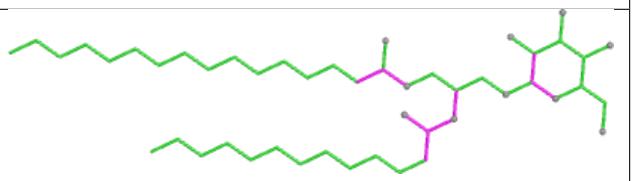


Rings

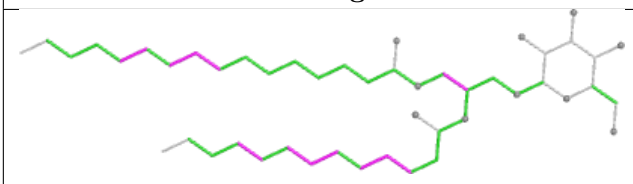
Ligand LMG D 401



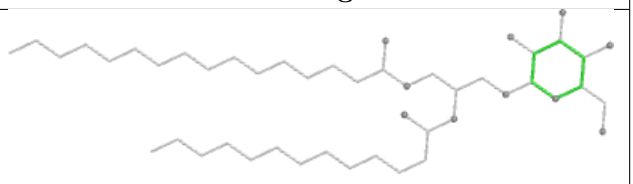
Bond lengths



Bond angles

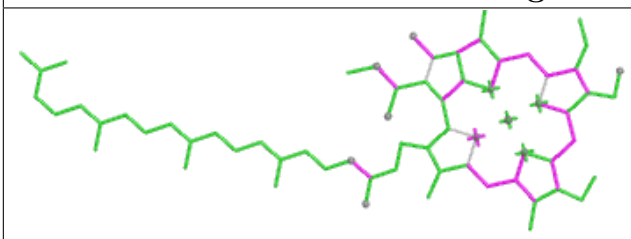


Torsions

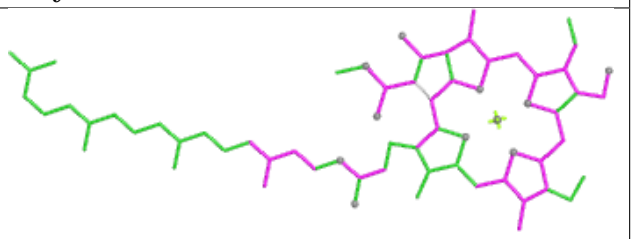


Rings

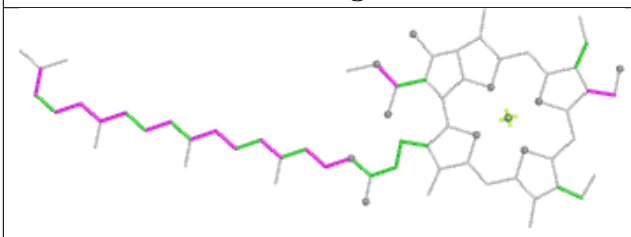
Ligand CHL y 313



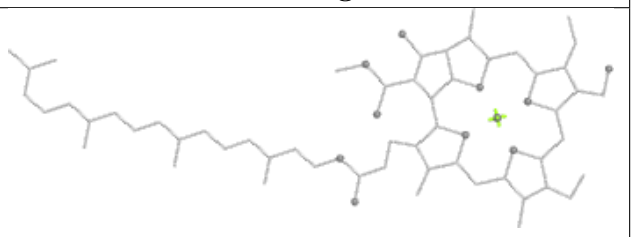
Bond lengths



Bond angles

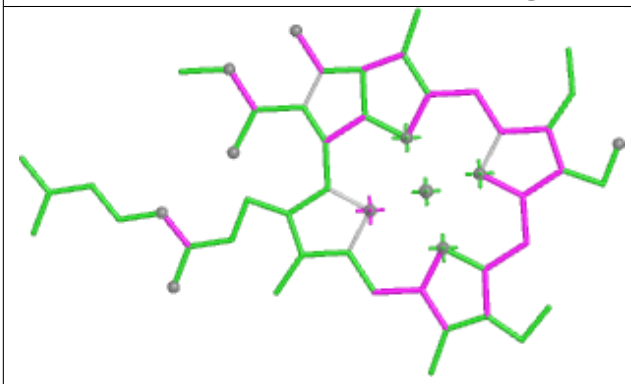


Torsions

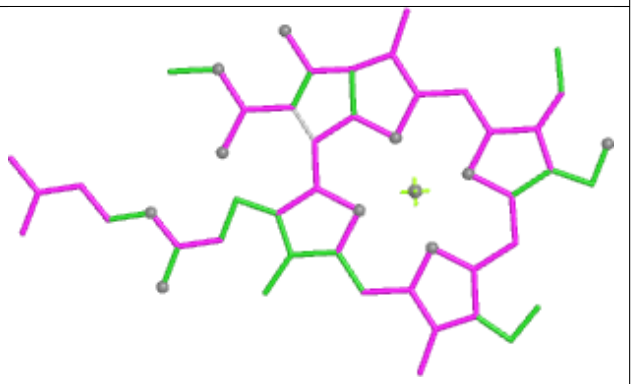


Rings

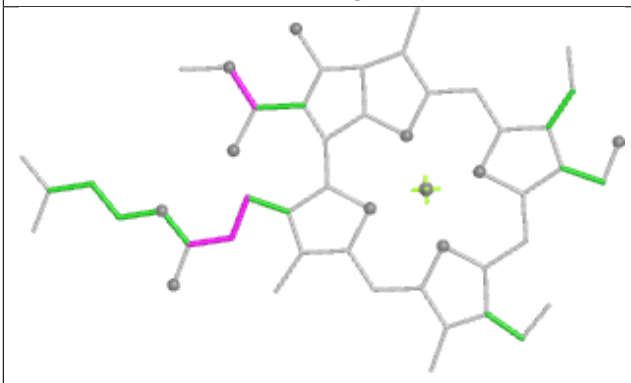
Ligand CHL G 312



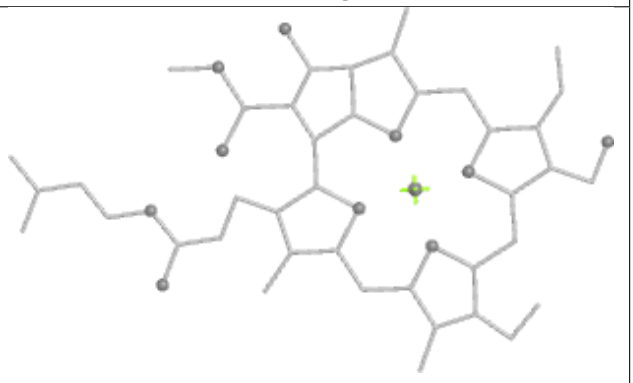
Bond lengths



Bond angles

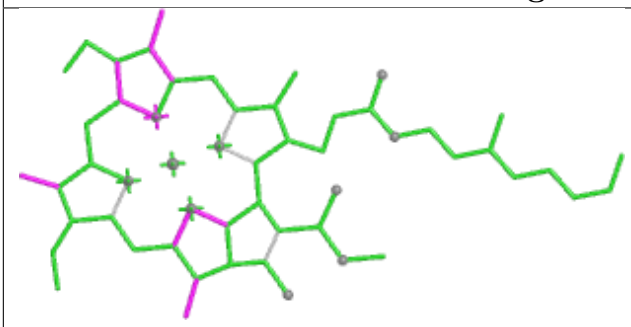


Torsions

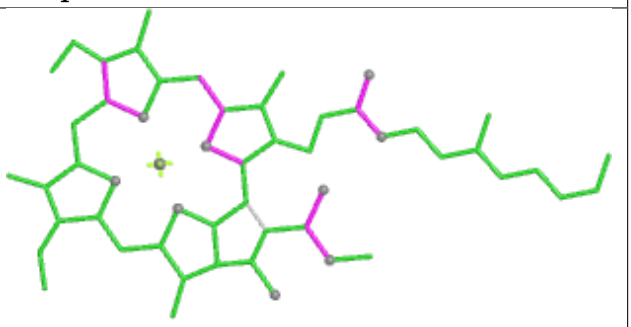


Rings

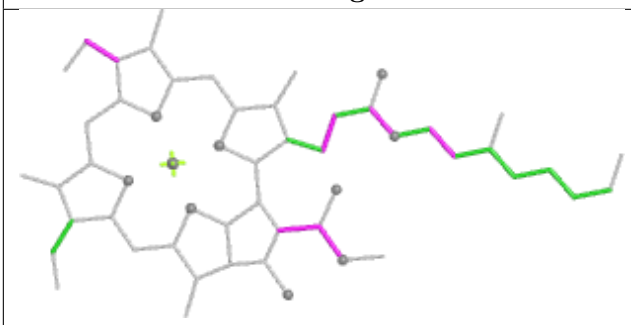
Ligand CLA q 305



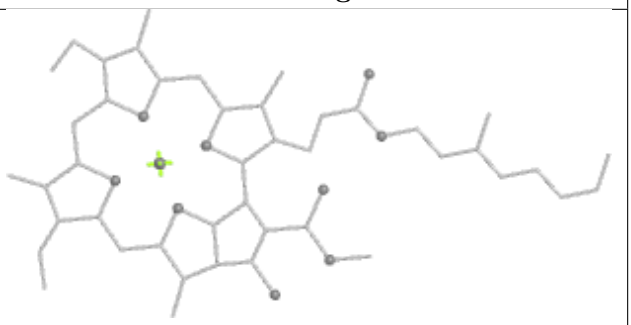
Bond lengths



Bond angles

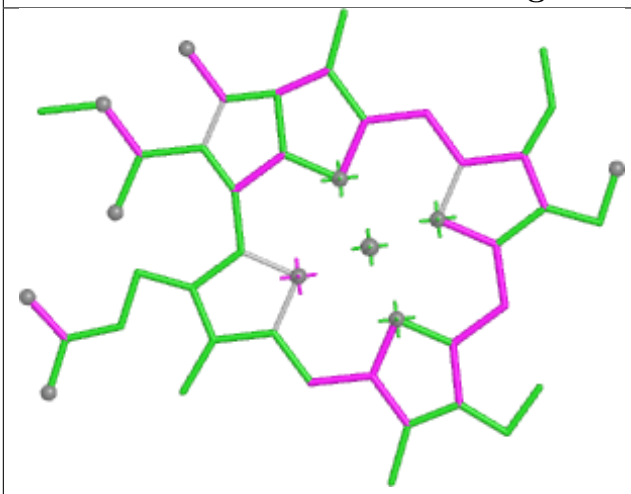


Torsions

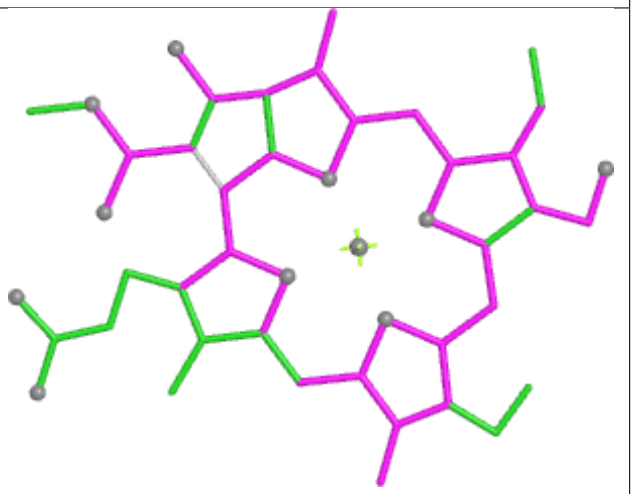


Rings

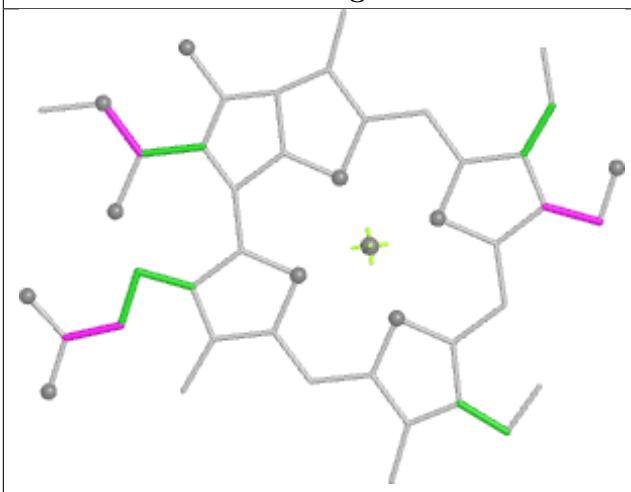
Ligand CHL 4 312



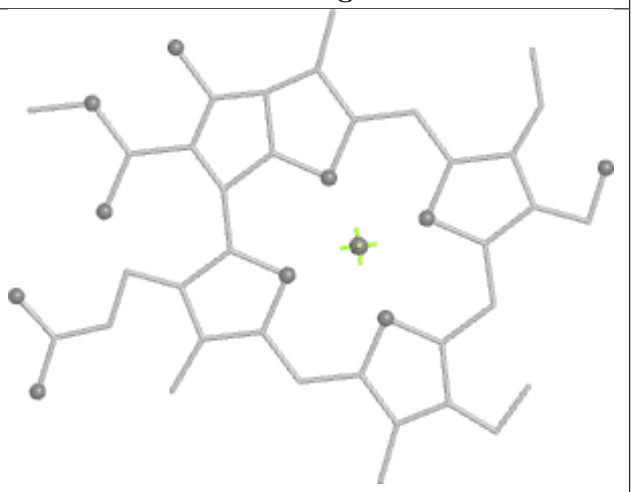
Bond lengths



Bond angles

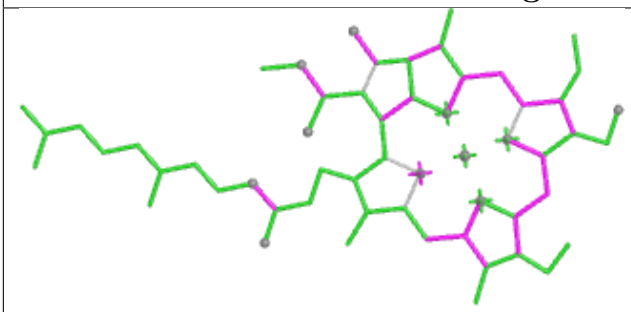


Torsions

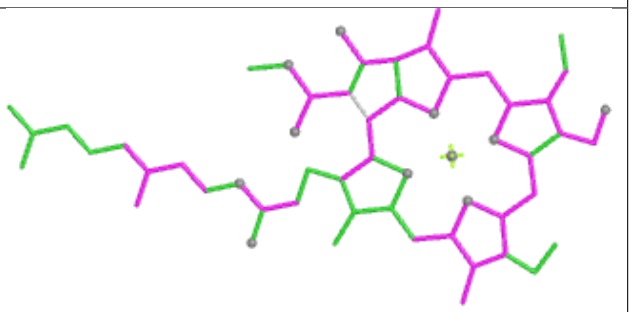


Rings

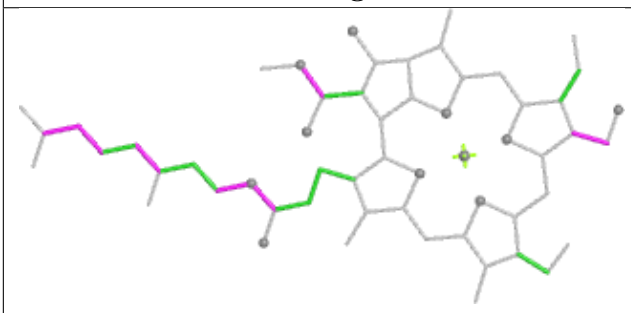
Ligand CHL N 312



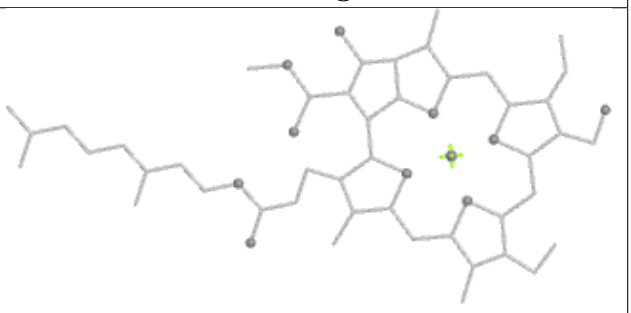
Bond lengths



Bond angles

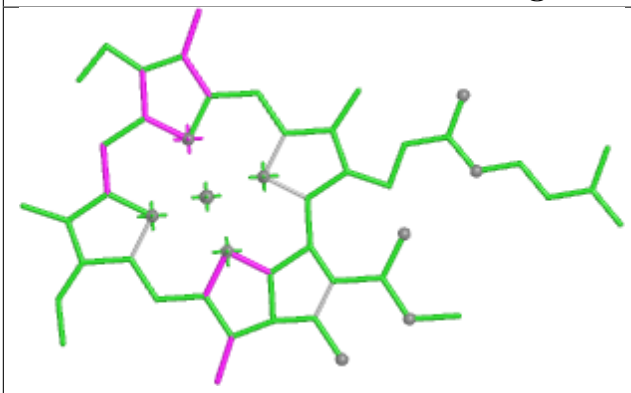


Torsions

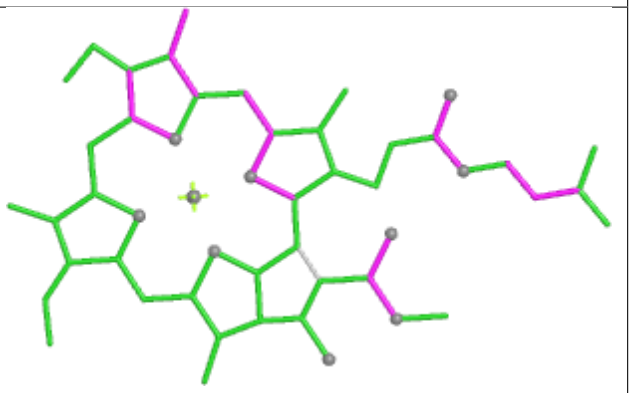


Rings

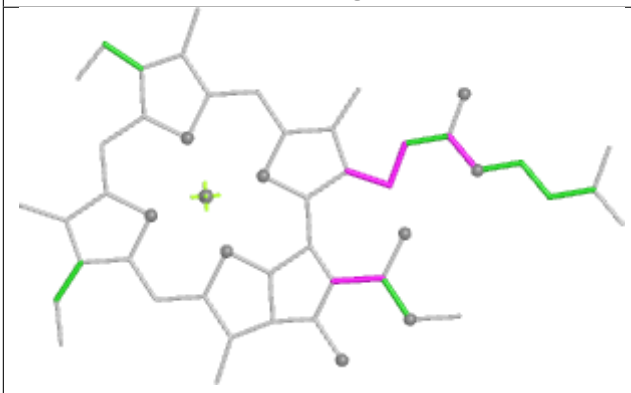
Ligand CLA 8 306



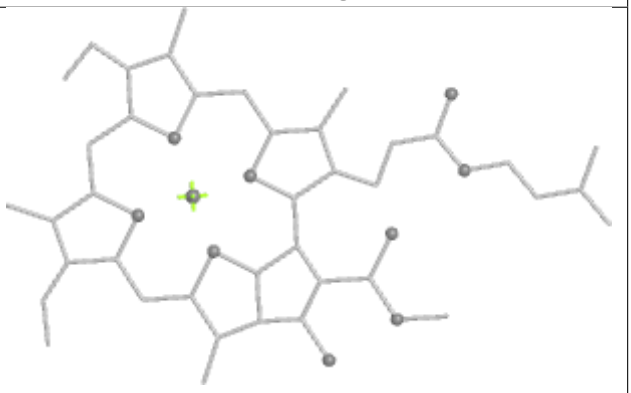
Bond lengths



Bond angles

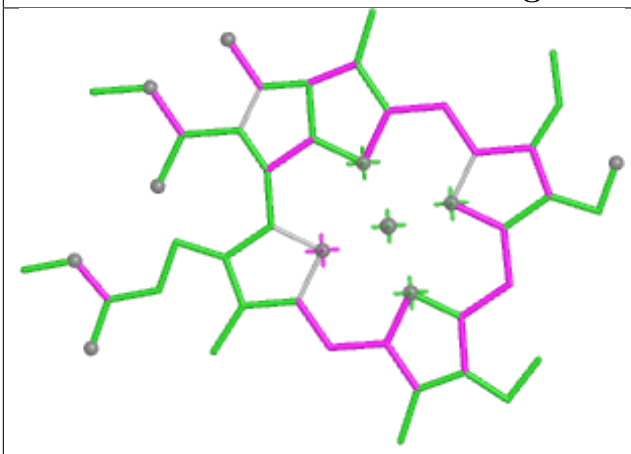


Torsions

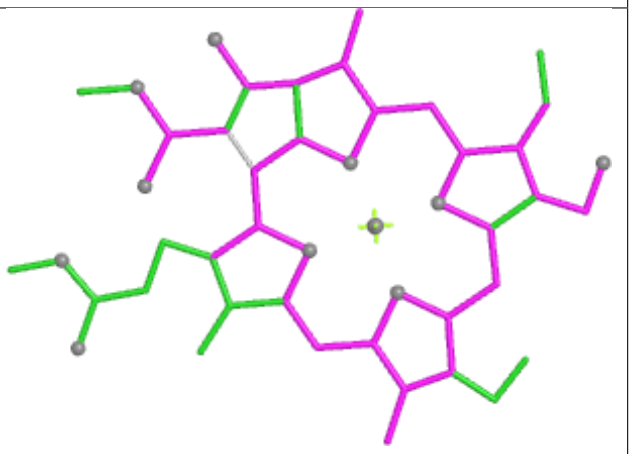


Rings

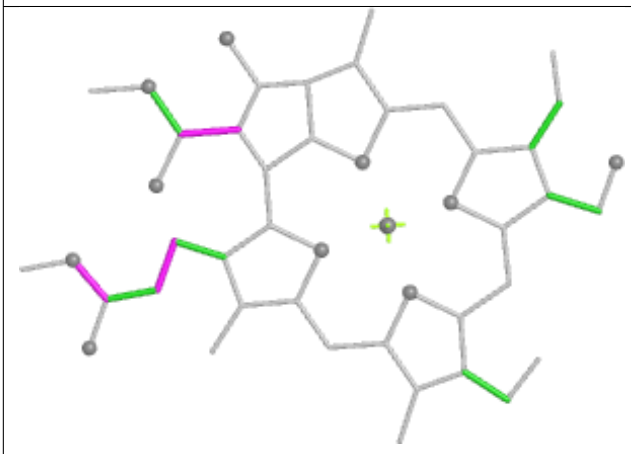
Ligand CHL R 602



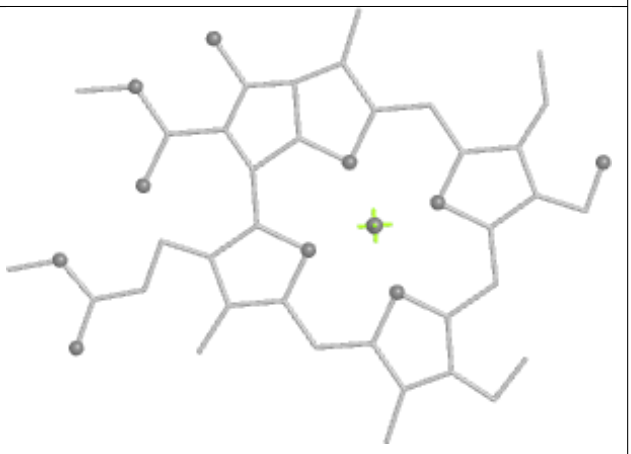
Bond lengths



Bond angles

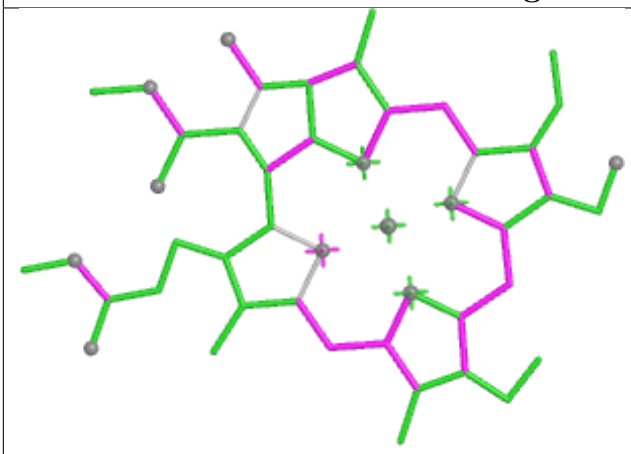


Torsions

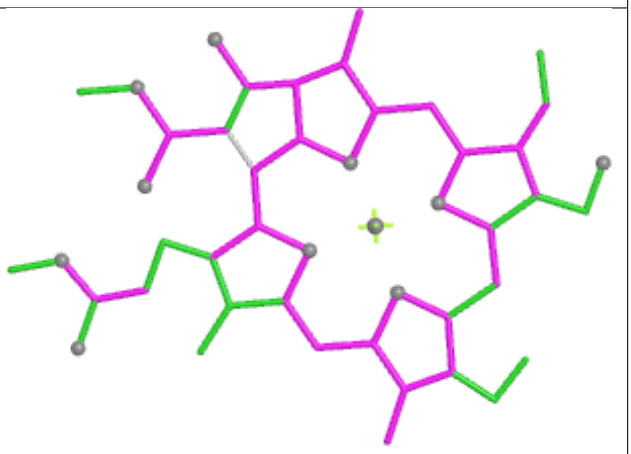


Rings

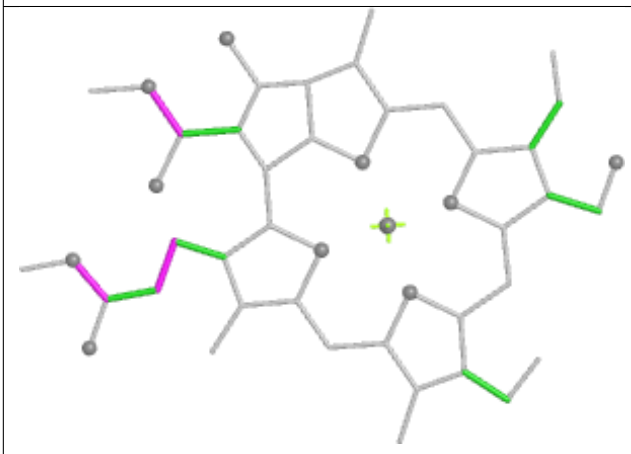
Ligand CHL Y 309



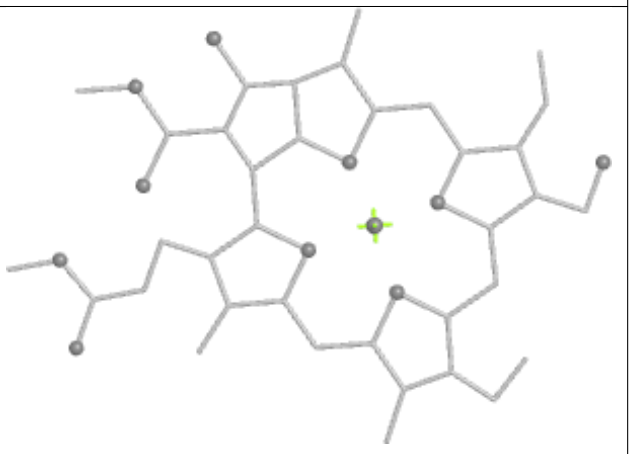
Bond lengths



Bond angles

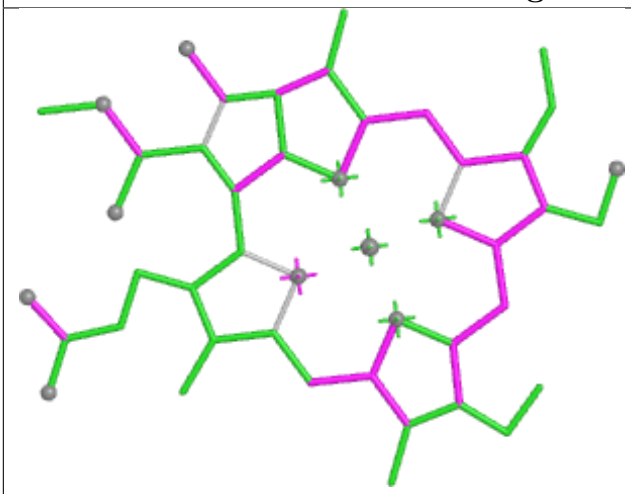


Torsions

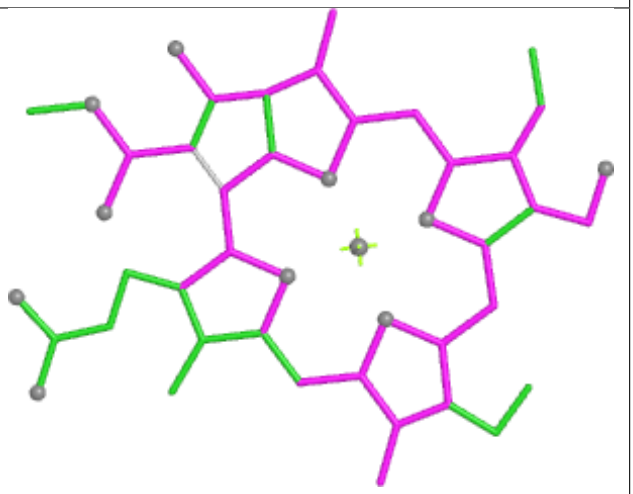


Rings

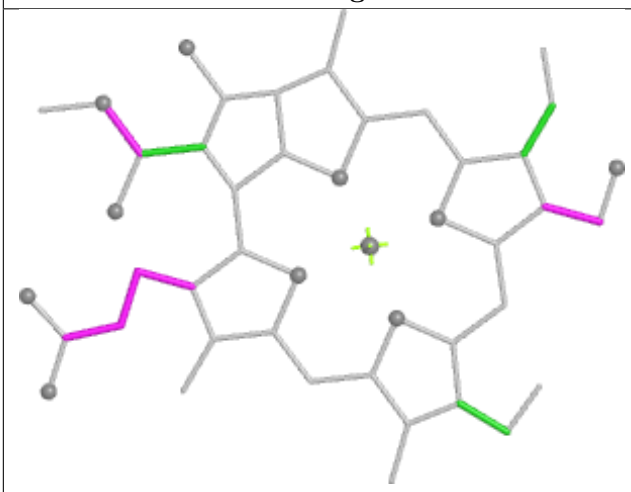
Ligand CHL u 310



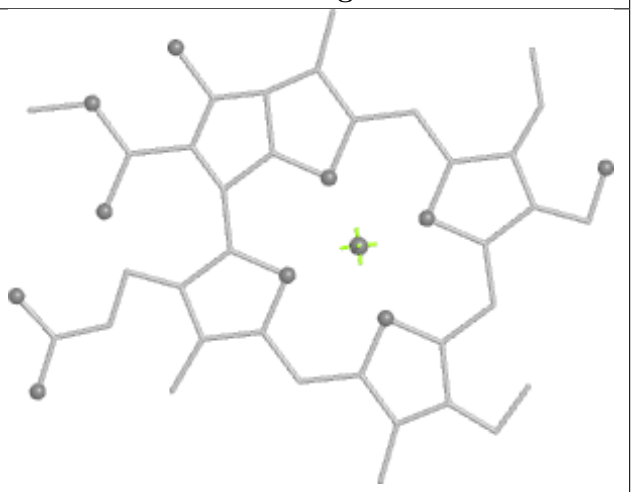
Bond lengths



Bond angles



Torsions

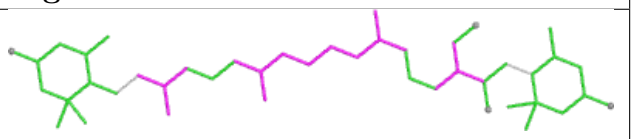


Rings

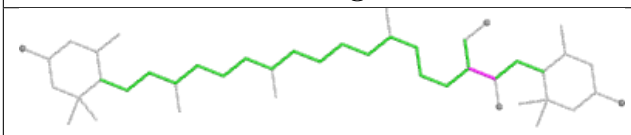
Ligand 0IE g 302



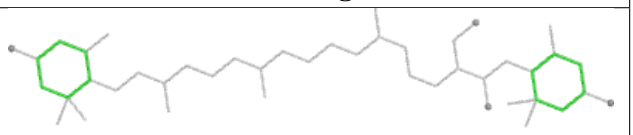
Bond lengths



Bond angles

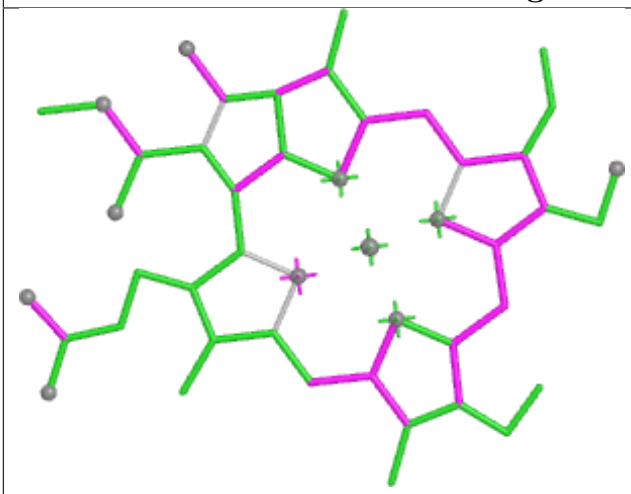


Torsions

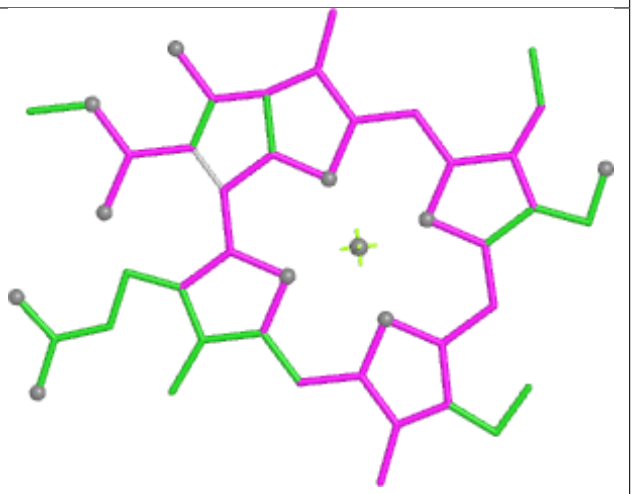


Rings

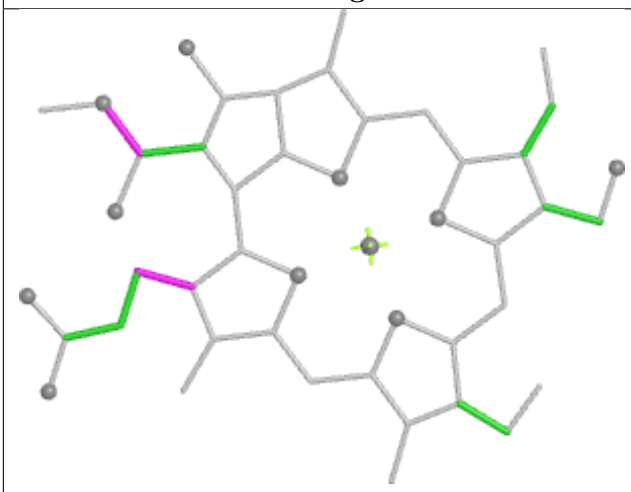
Ligand CHL u 311



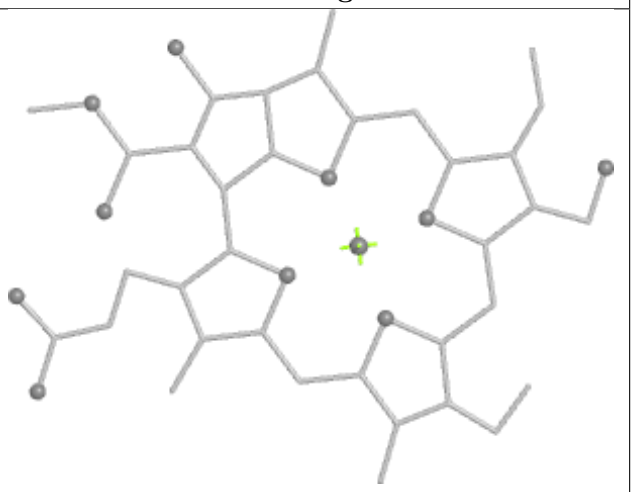
Bond lengths



Bond angles

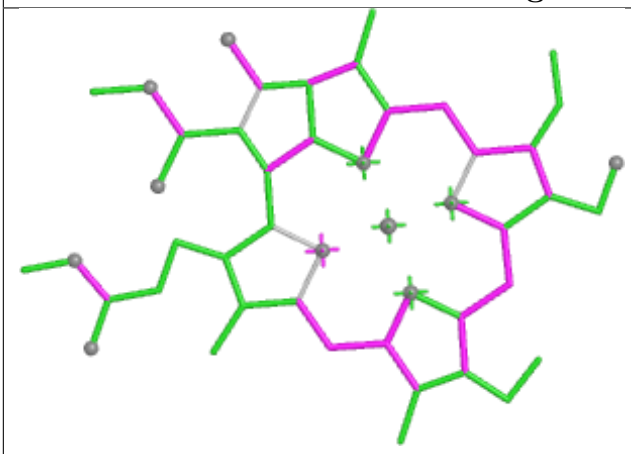


Torsions

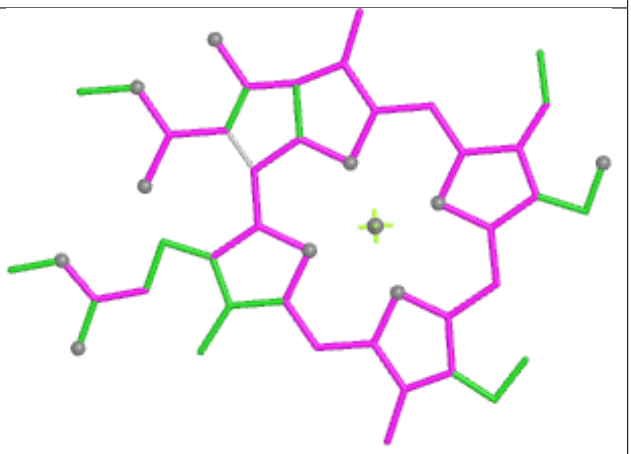


Rings

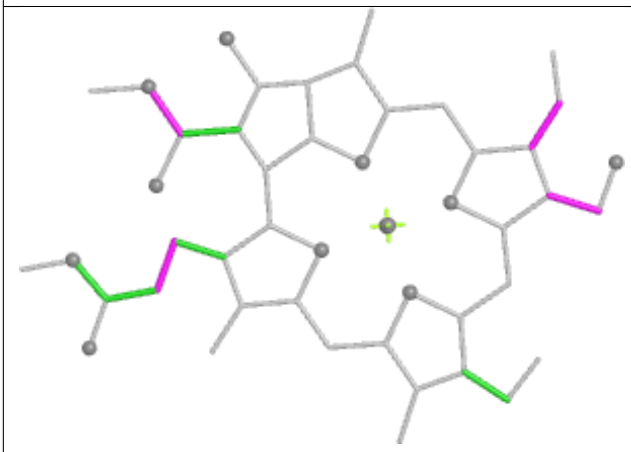
Ligand CHL S 608



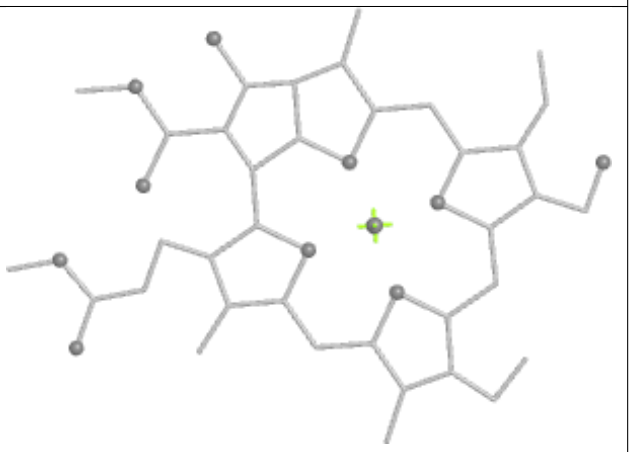
Bond lengths



Bond angles

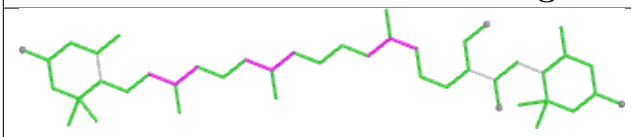


Torsions

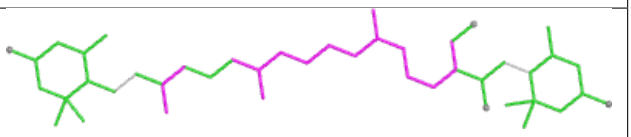


Rings

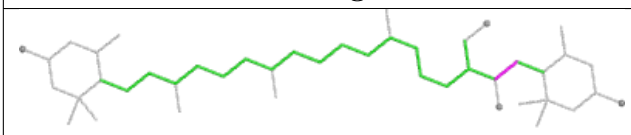
Ligand 0IE 3 303



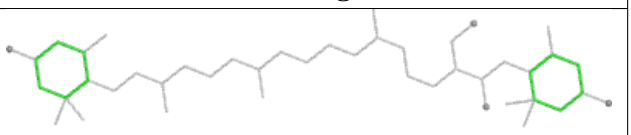
Bond lengths



Bond angles

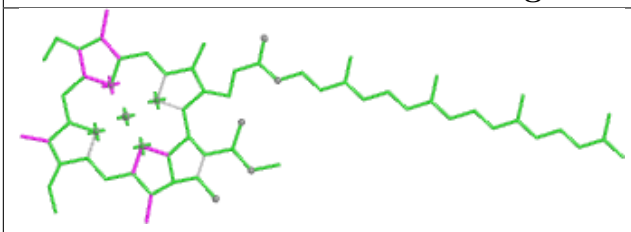


Torsions

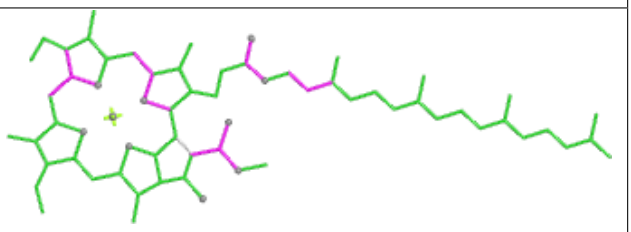


Rings

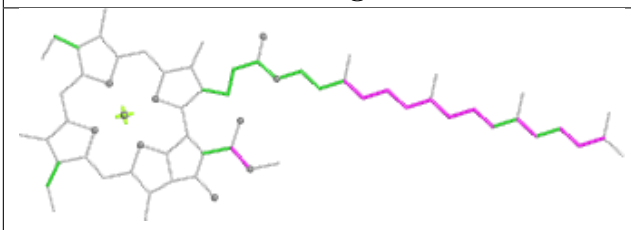
Ligand CLA B 609



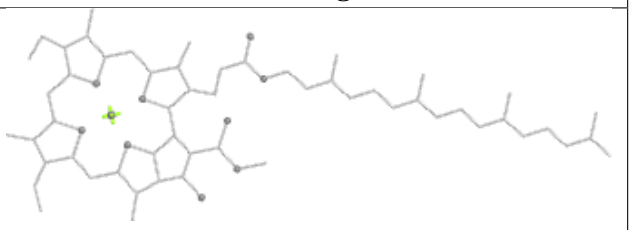
Bond lengths



Bond angles



Torsions



Rings

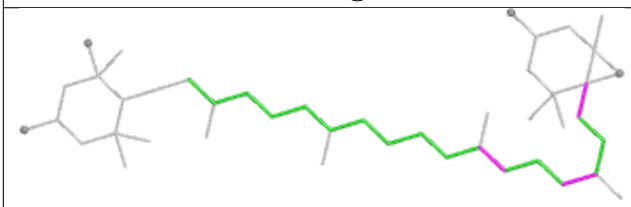
Ligand NEX 5 304



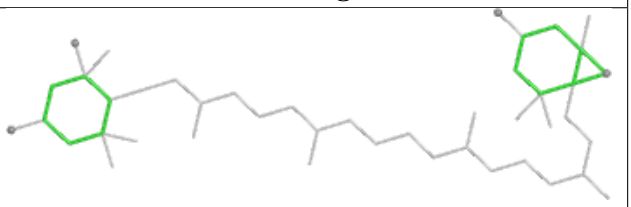
Bond lengths



Bond angles

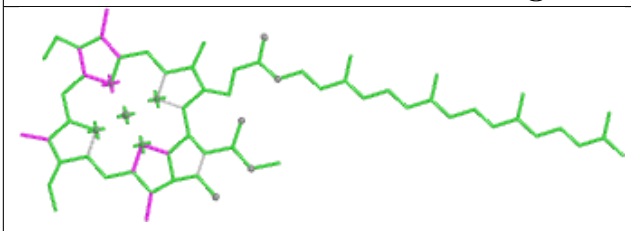


Torsions

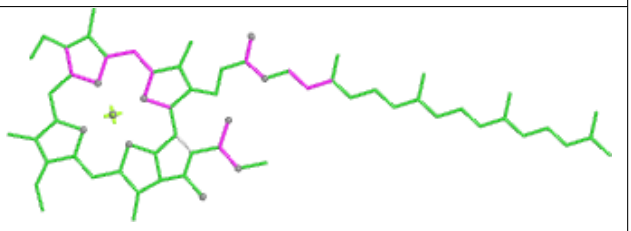


Rings

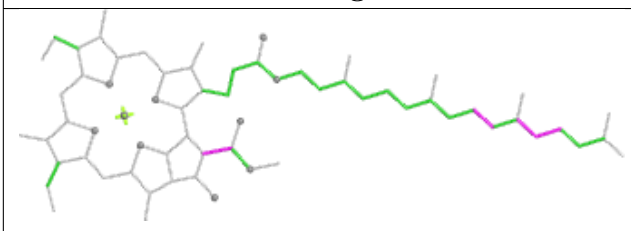
Ligand CLA b 611



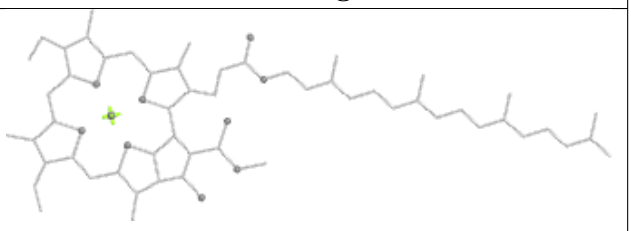
Bond lengths



Bond angles

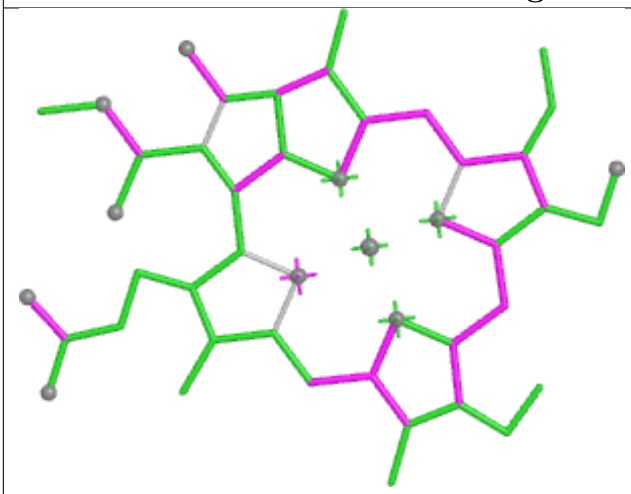


Torsions

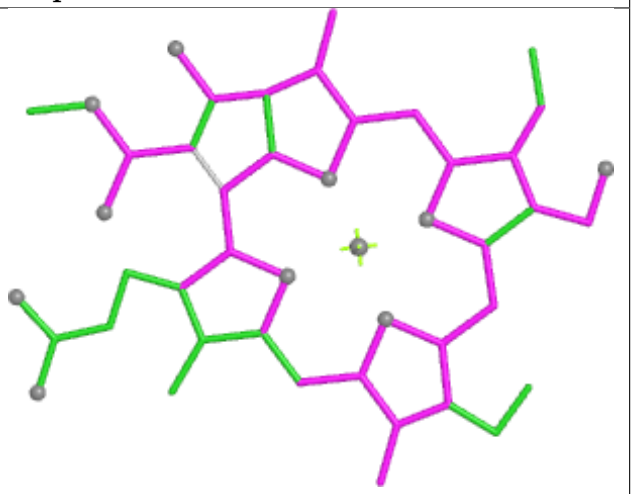


Rings

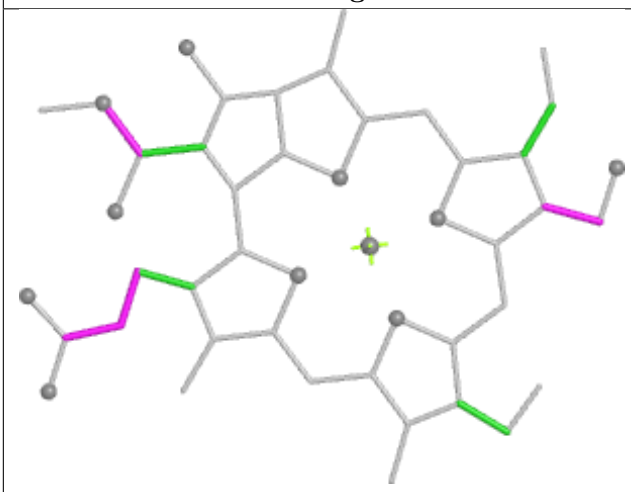
Ligand CHL p 310



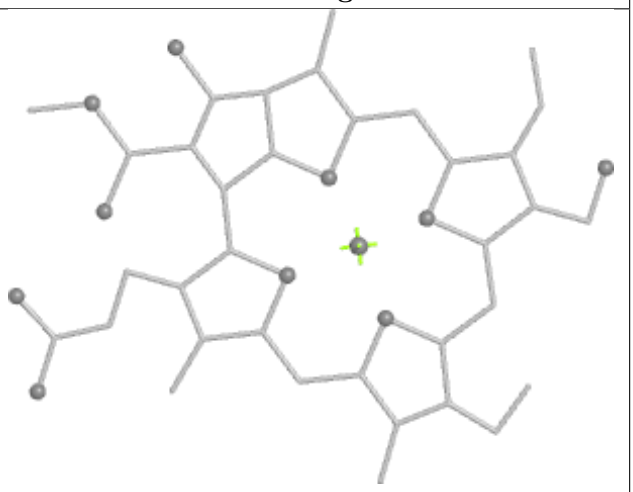
Bond lengths



Bond angles

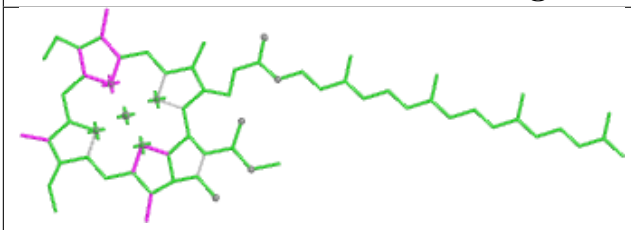


Torsions

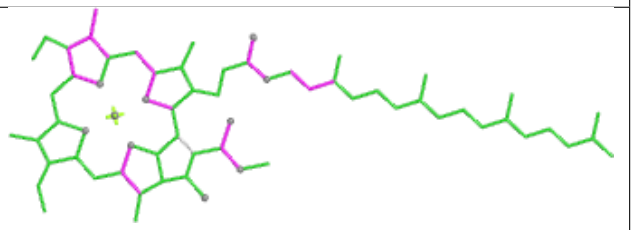


Rings

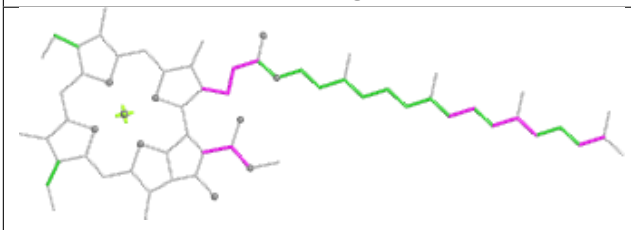
Ligand CLA c 601



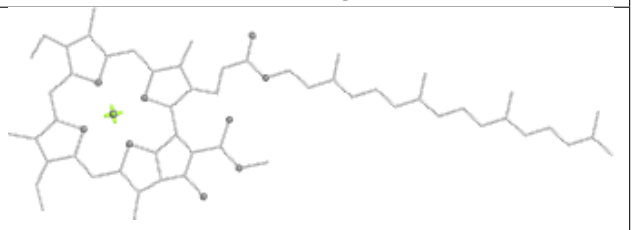
Bond lengths



Bond angles

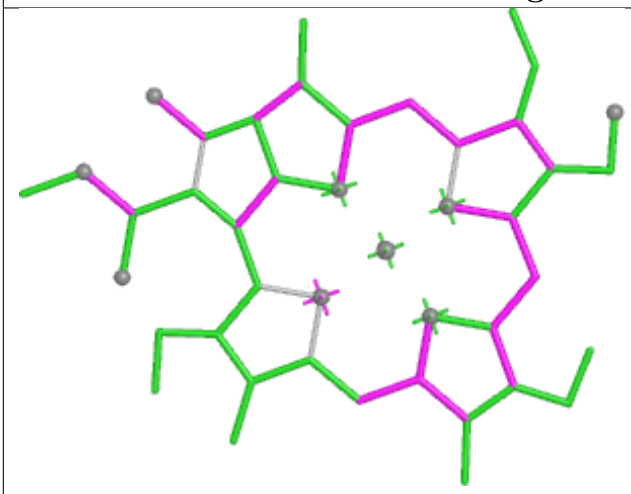


Torsions

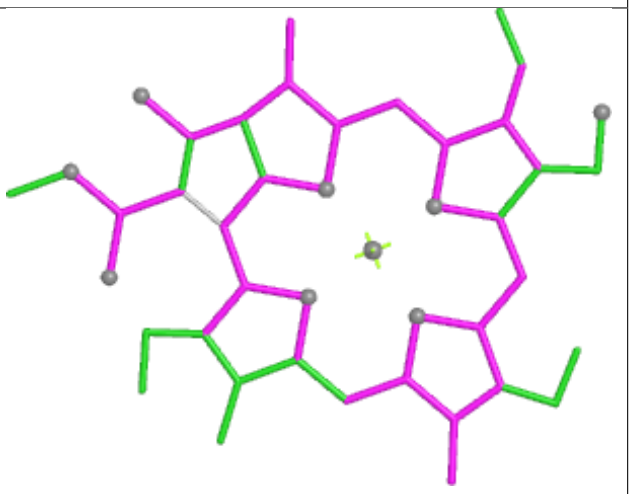


Rings

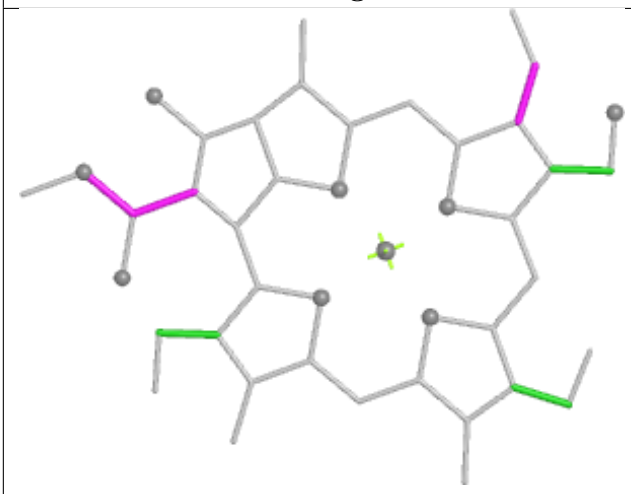
Ligand CHL u 313



Bond lengths



Bond angles

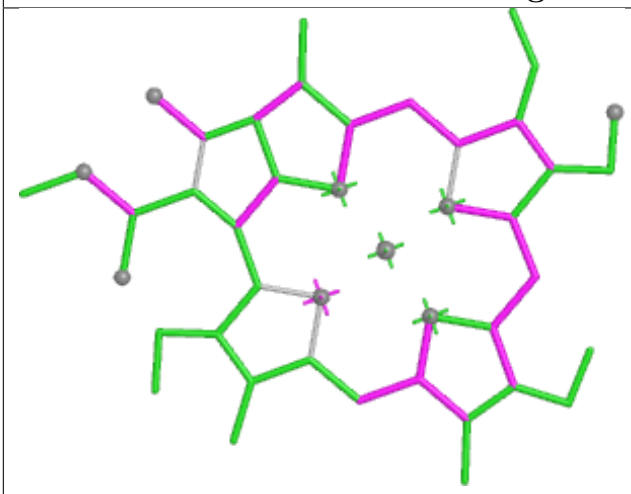


Torsions

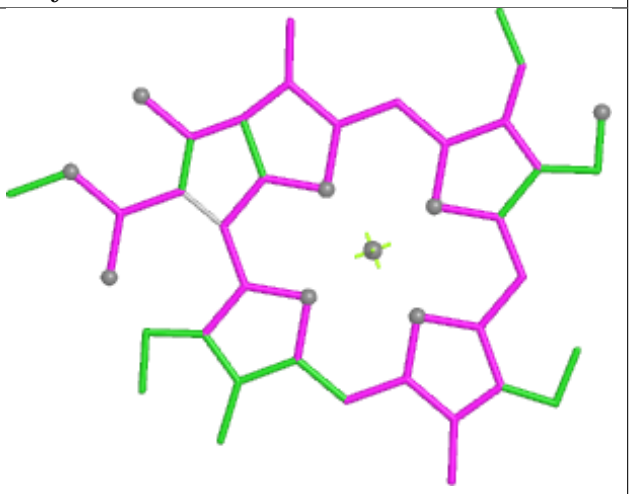


Rings

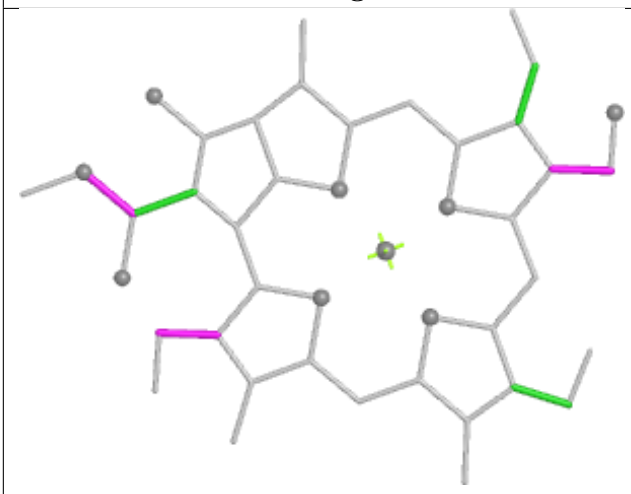
Ligand CHL y 309



Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 d 406



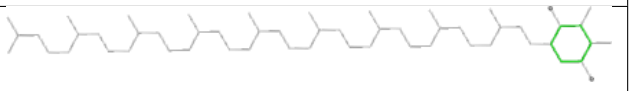
Bond lengths



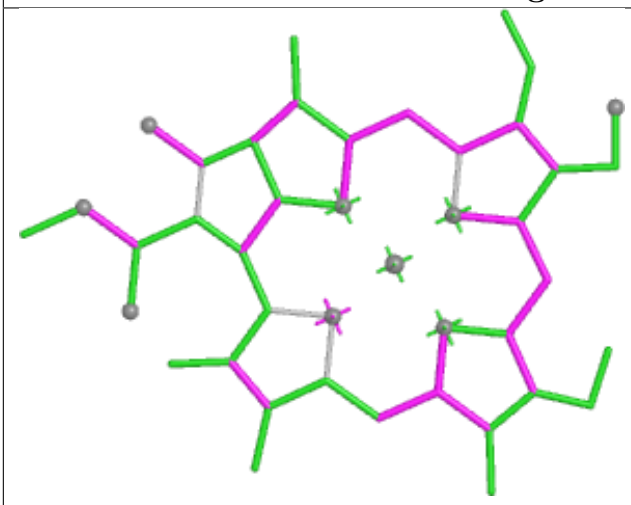
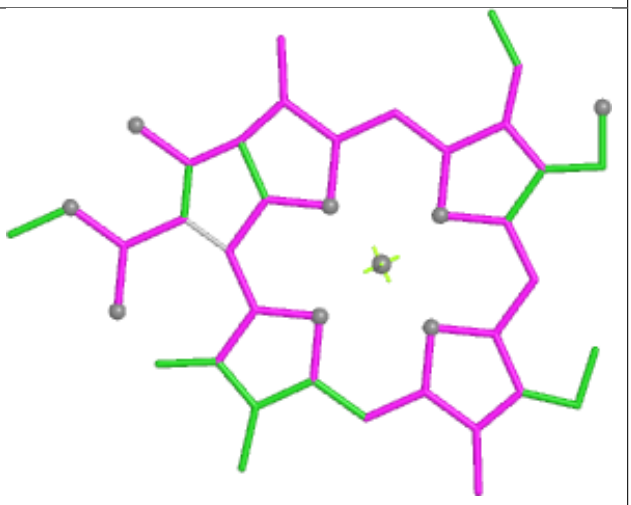
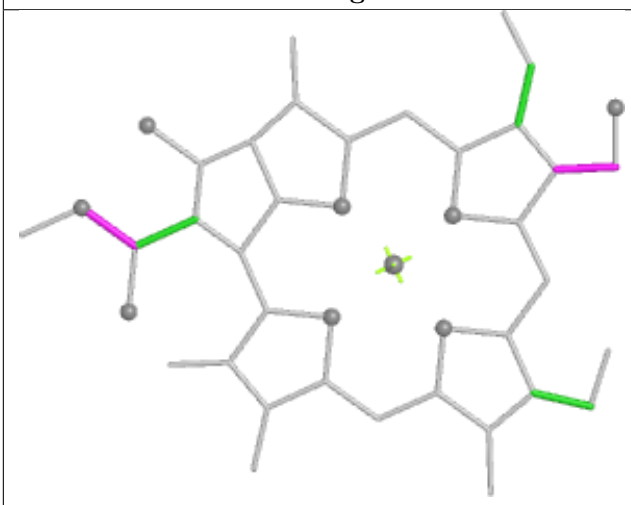
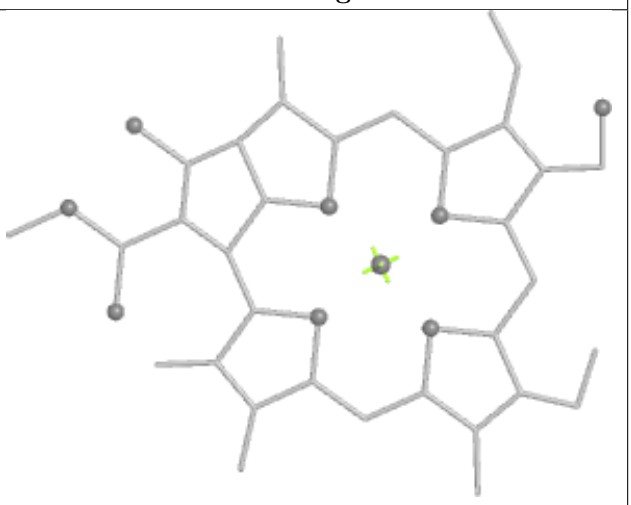
Bond angles

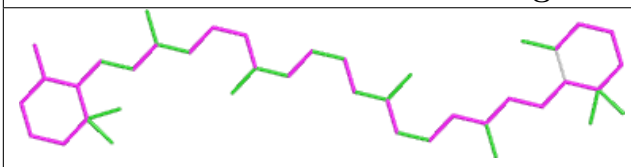
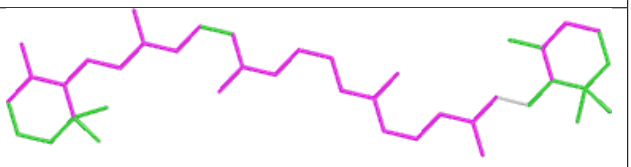
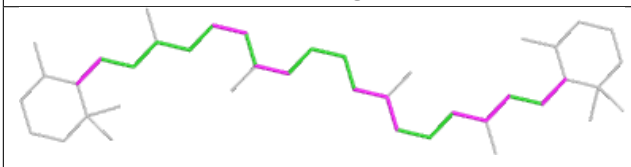
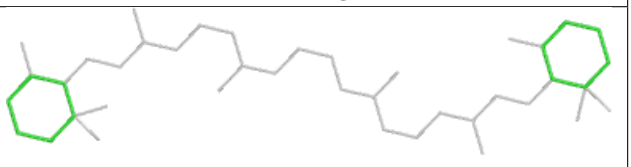


Torsions

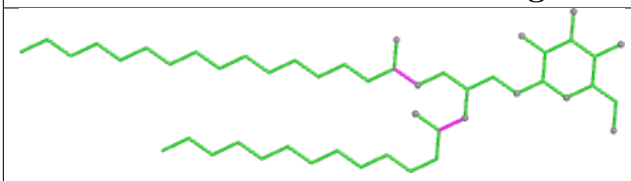


Rings

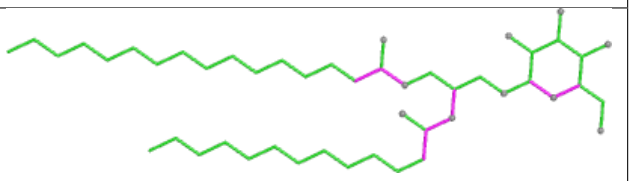
Ligand CHL 5 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT s 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

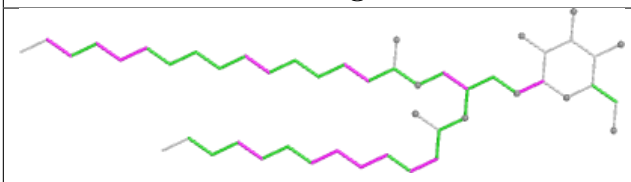
Ligand LMG i 101



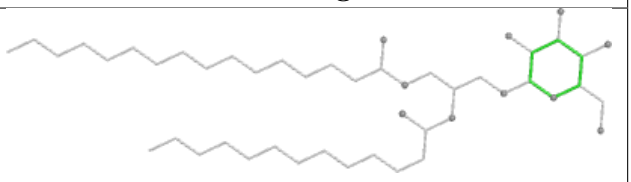
Bond lengths



Bond angles

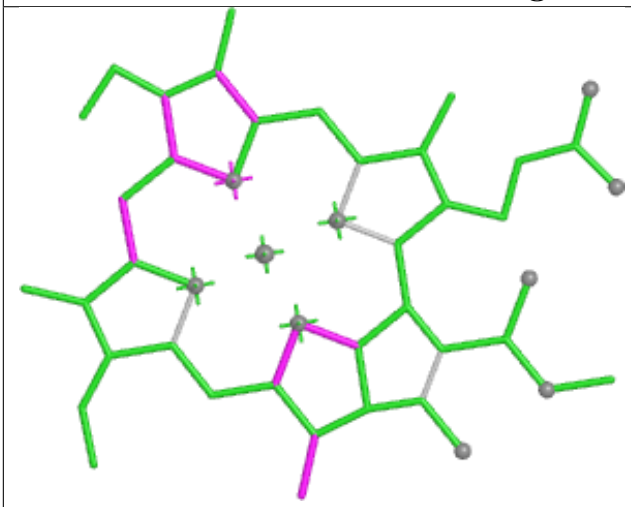


Torsions

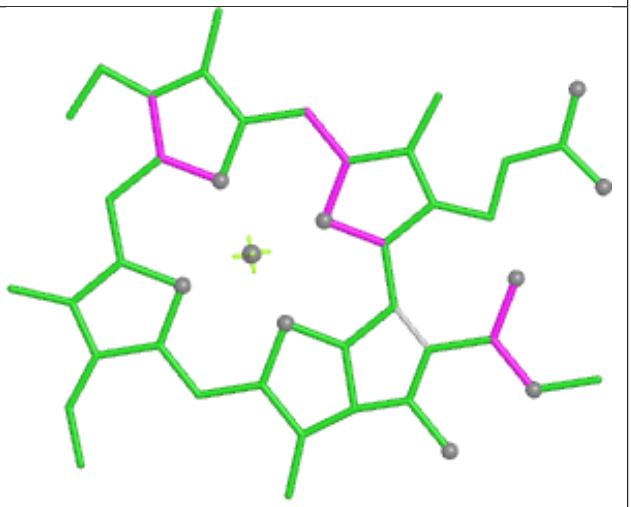


Rings

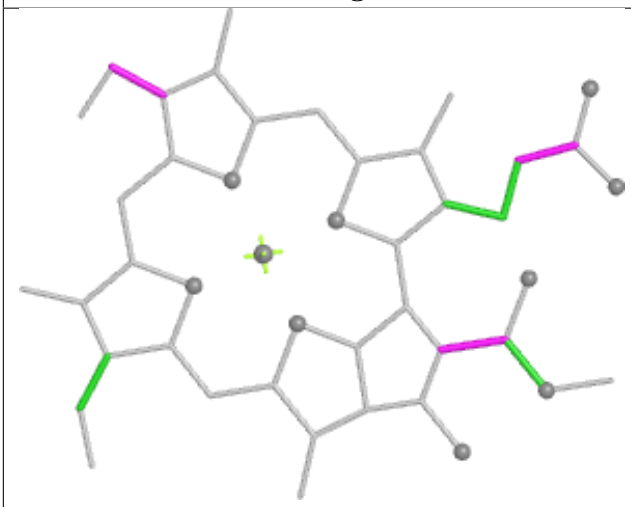
Ligand CLA 9 315



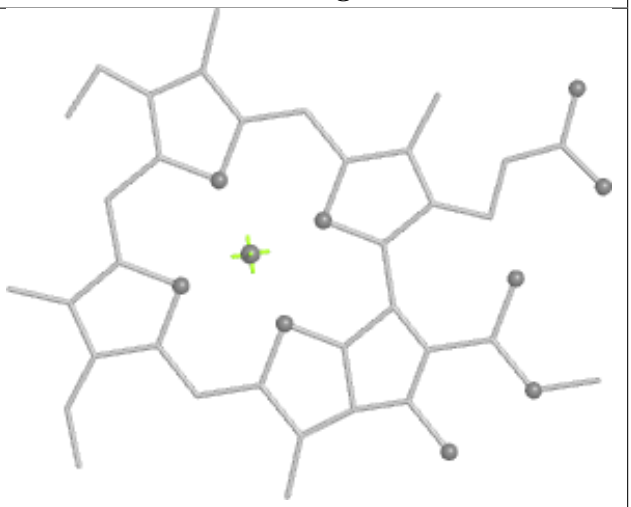
Bond lengths



Bond angles

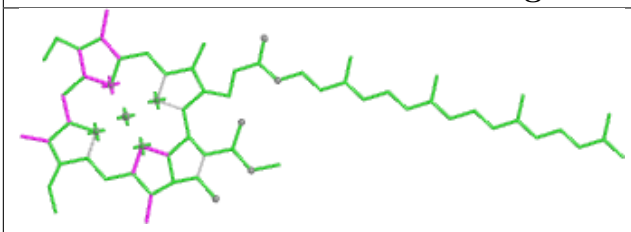


Torsions

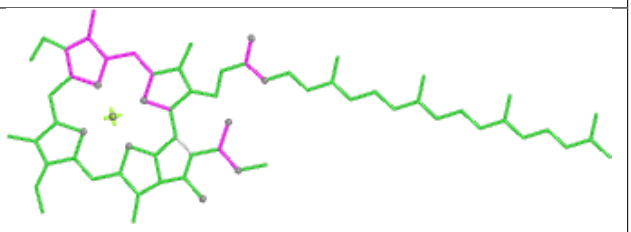


Rings

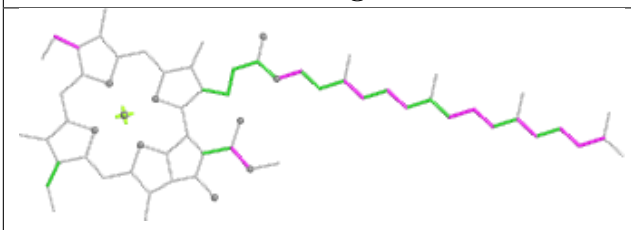
Ligand CLA C 603



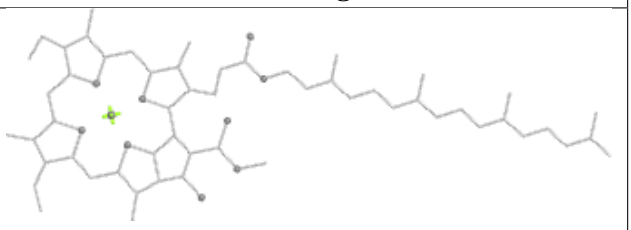
Bond lengths



Bond angles



Torsions



Rings

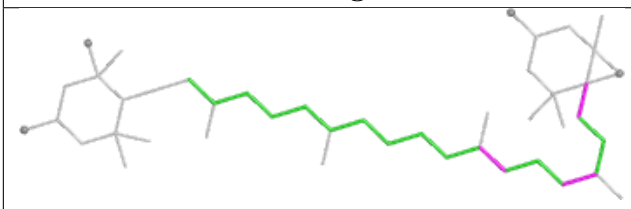
Ligand NEX 7 304



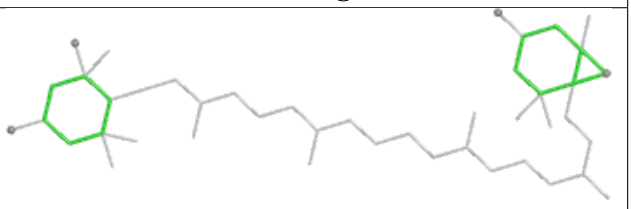
Bond lengths



Bond angles

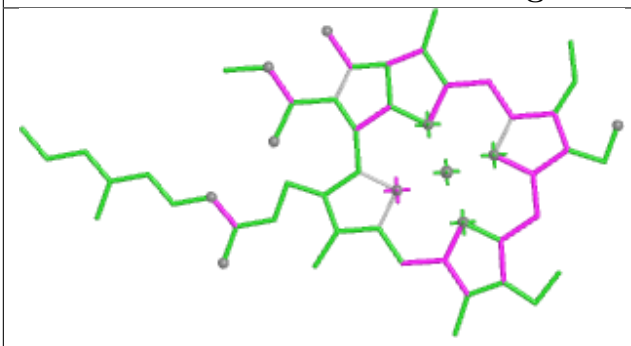


Torsions

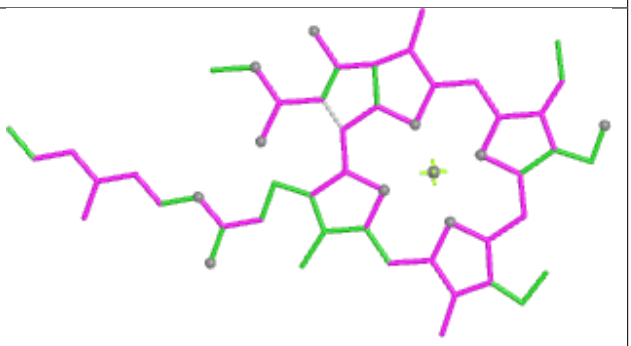


Rings

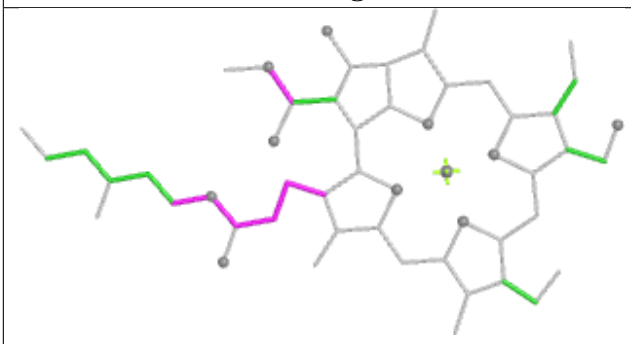
Ligand CHL n 310



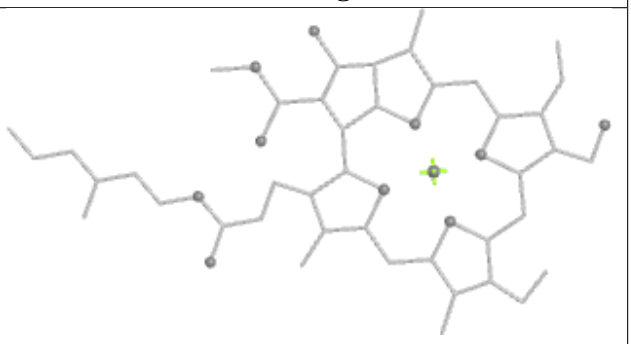
Bond lengths



Bond angles

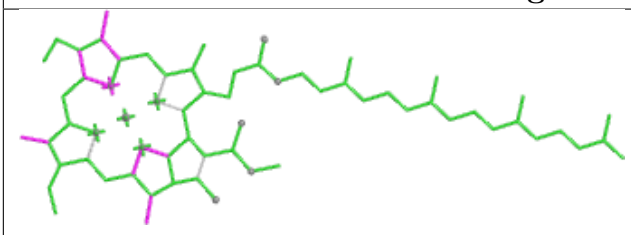


Torsions

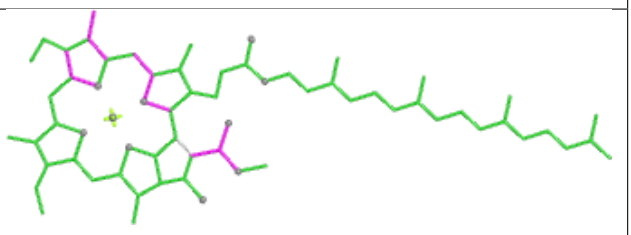


Rings

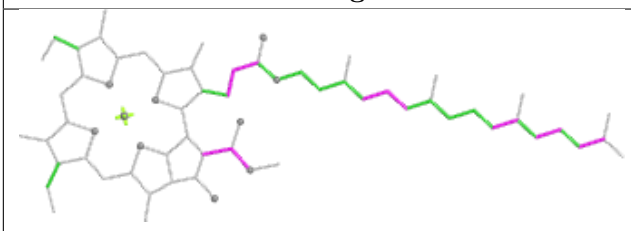
Ligand CLA b 602



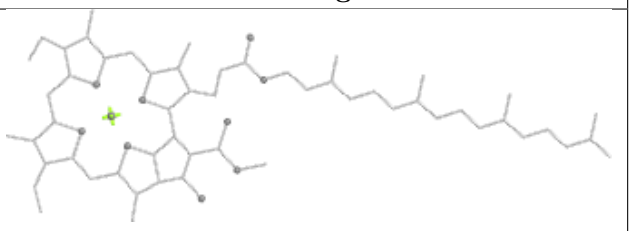
Bond lengths



Bond angles

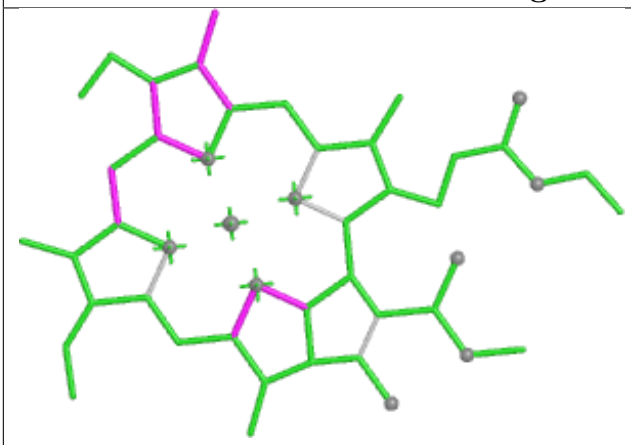


Torsions

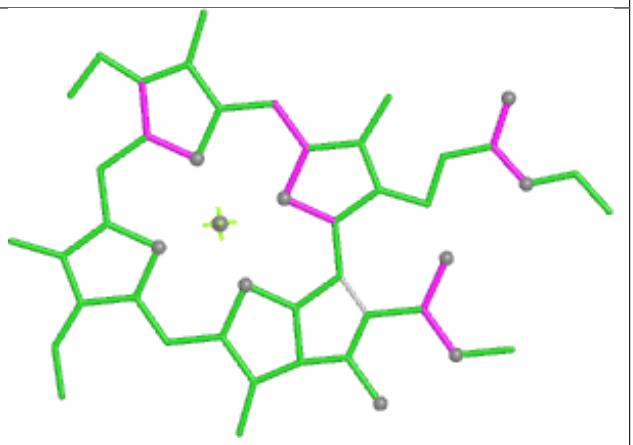


Rings

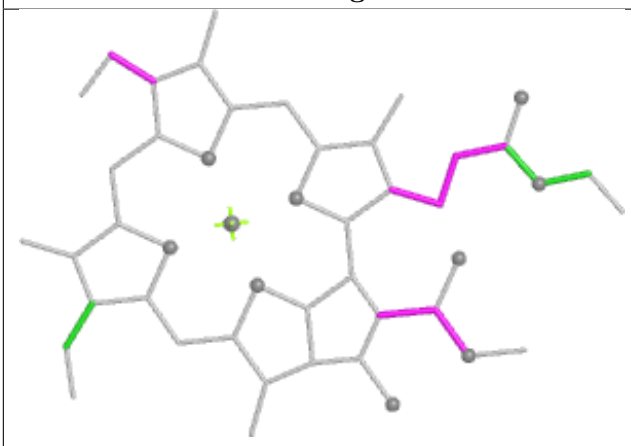
Ligand CLA r 314



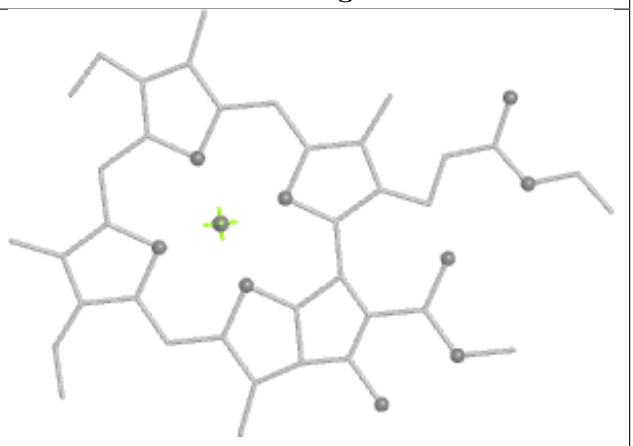
Bond lengths



Bond angles

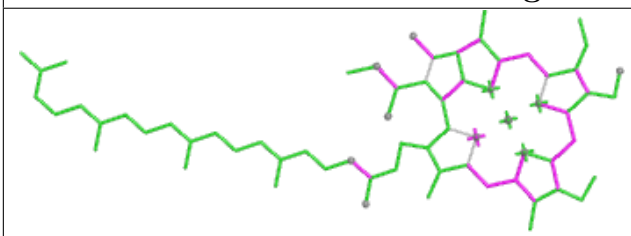


Torsions

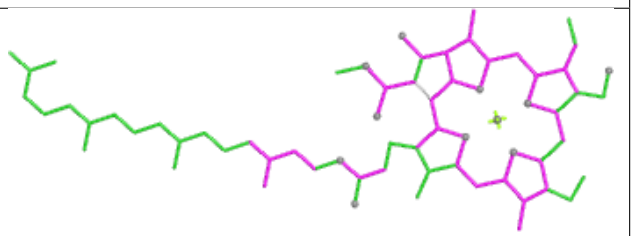


Rings

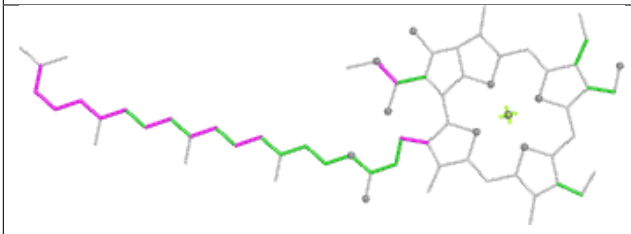
Ligand CHL Y 304



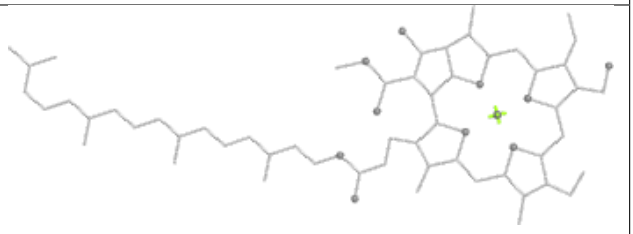
Bond lengths



Bond angles

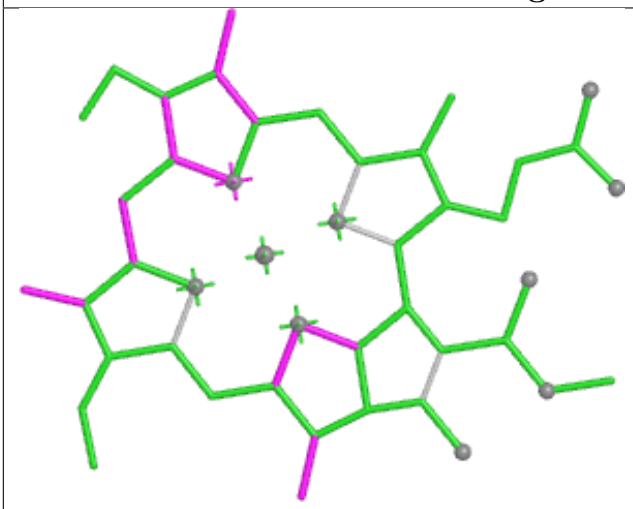


Torsions

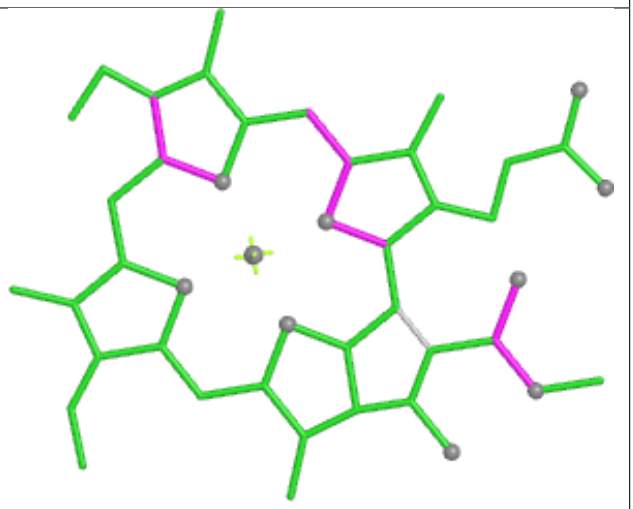


Rings

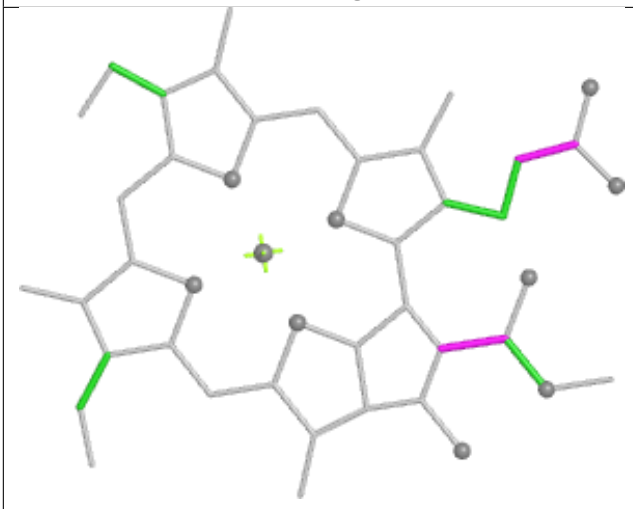
Ligand CLA 5 316



Bond lengths



Bond angles

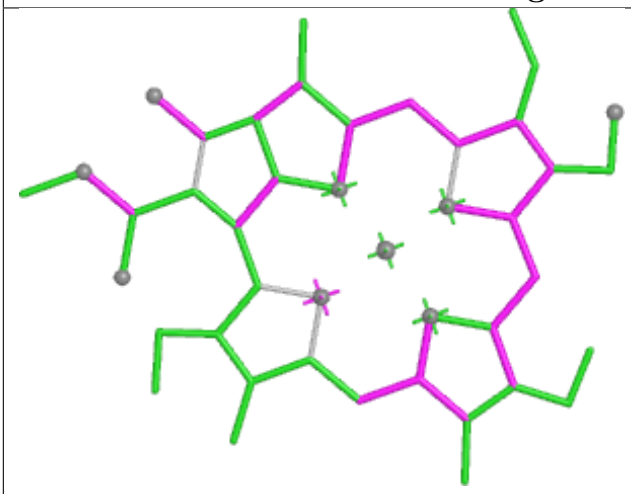


Torsions

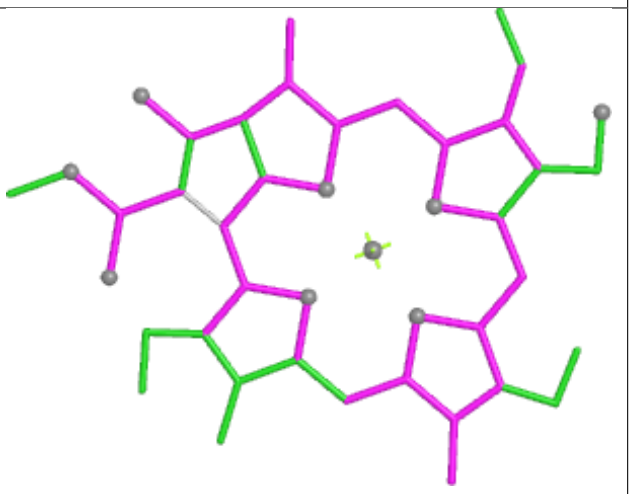


Rings

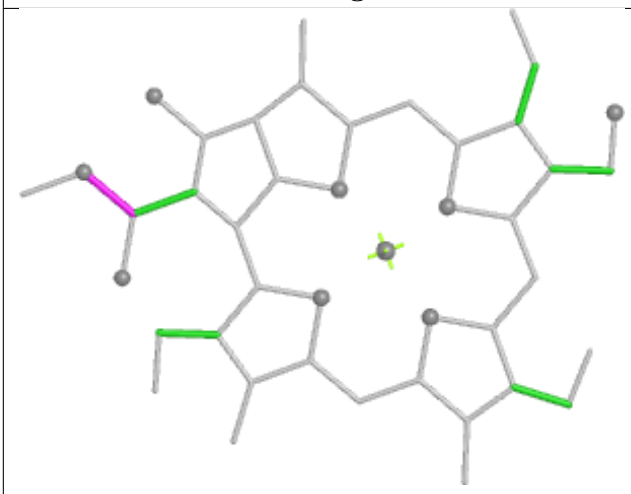
Ligand CHL 1 310



Bond lengths



Bond angles

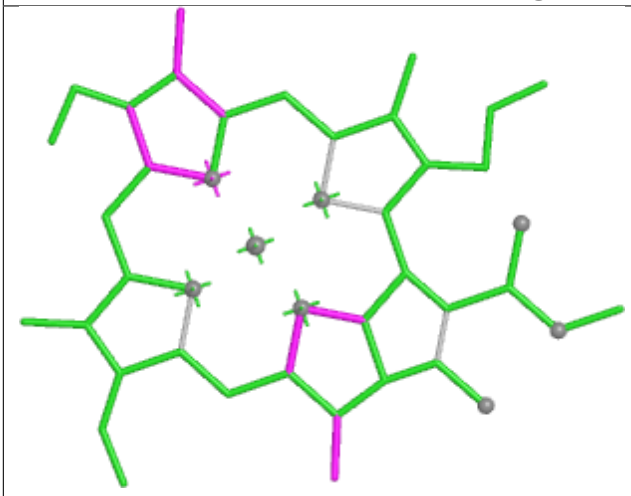


Torsions

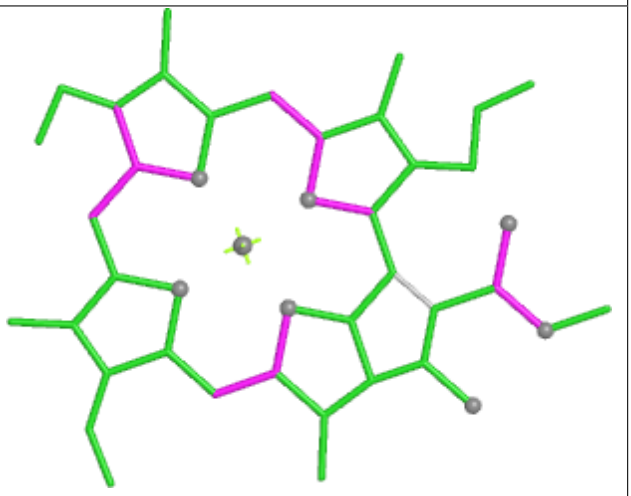


Rings

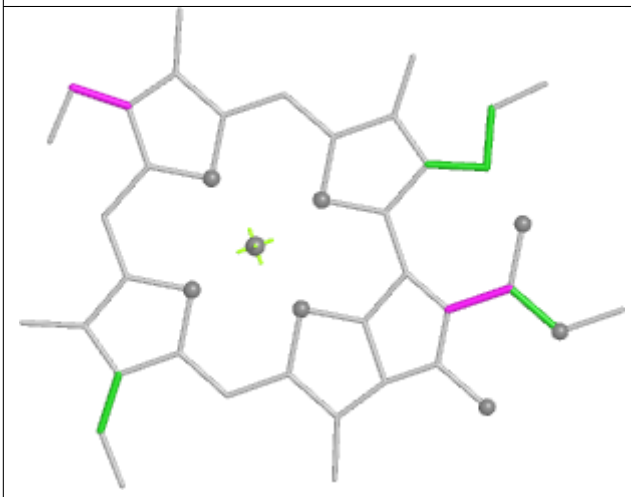
Ligand CLA s 405



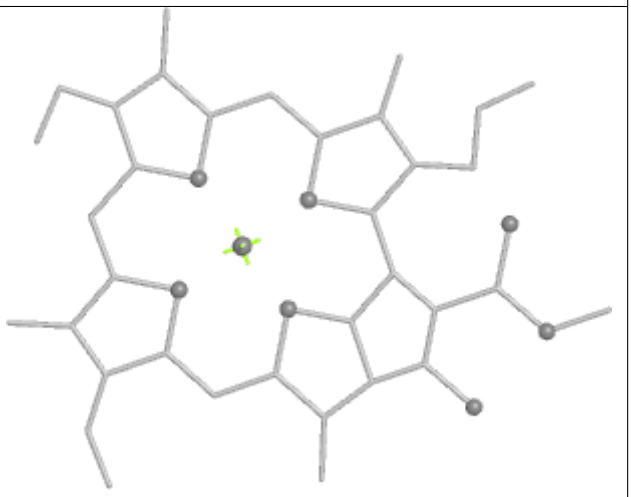
Bond lengths



Bond angles

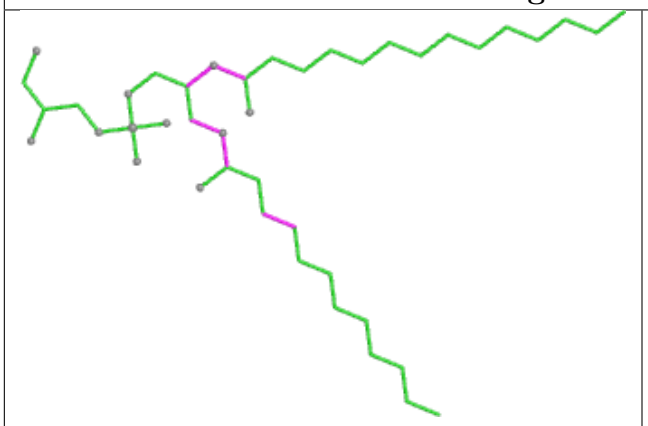


Torsions

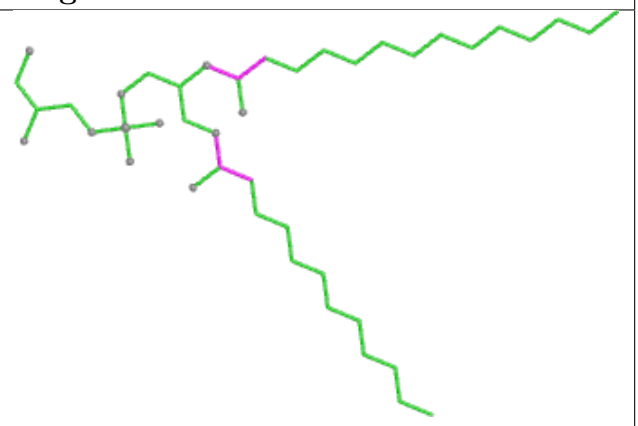


Rings

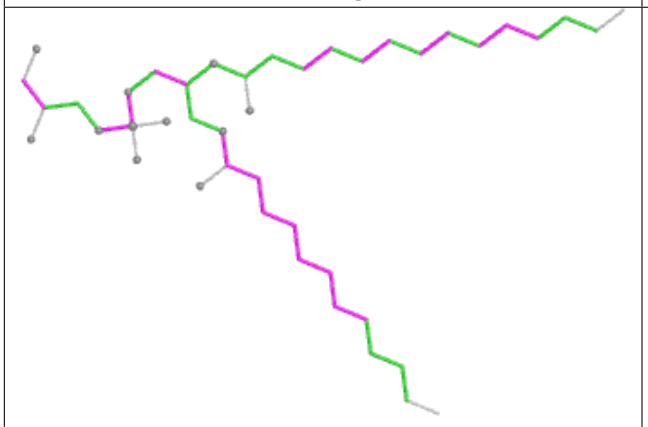
Ligand LHG g 319



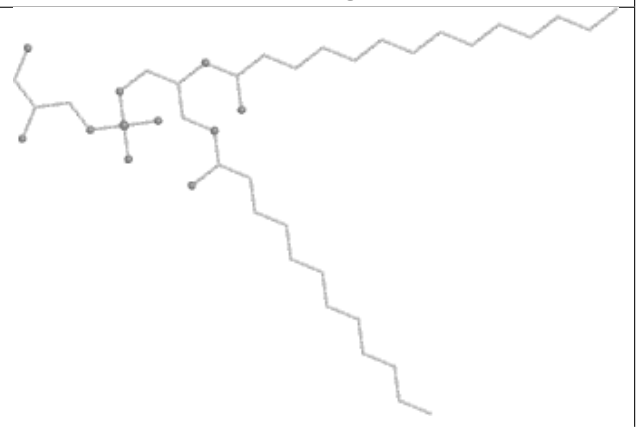
Bond lengths



Bond angles

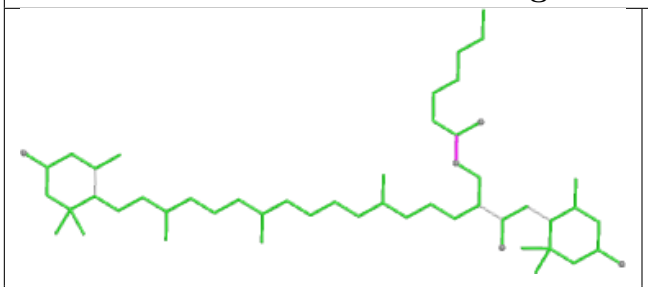


Torsions

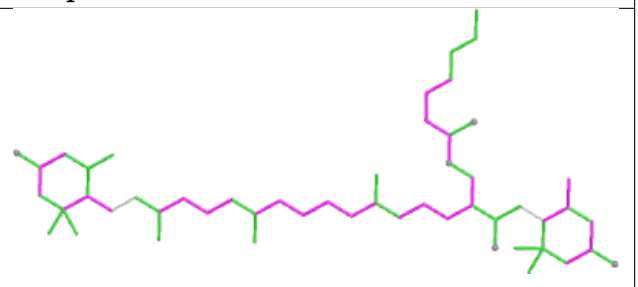


Rings

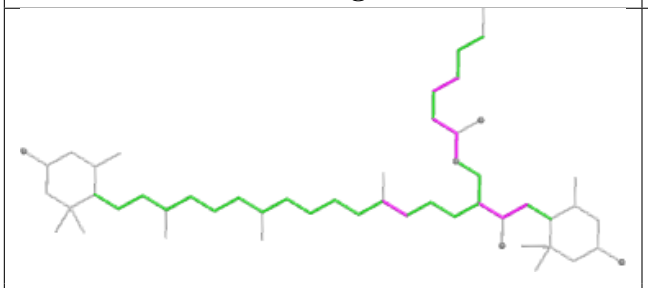
Ligand 0UR q 301



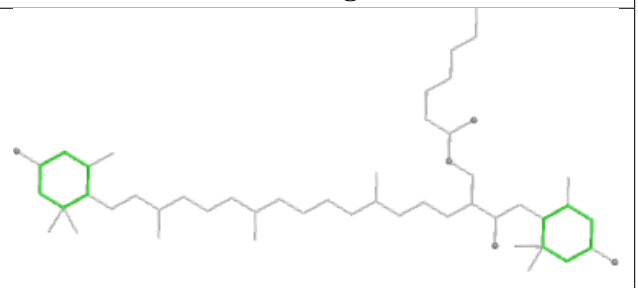
Bond lengths



Bond angles

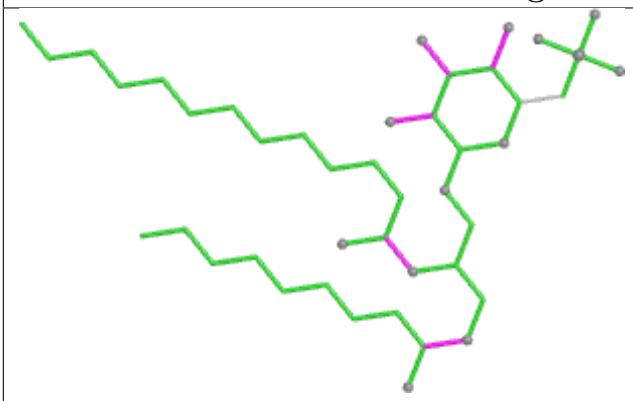


Torsions

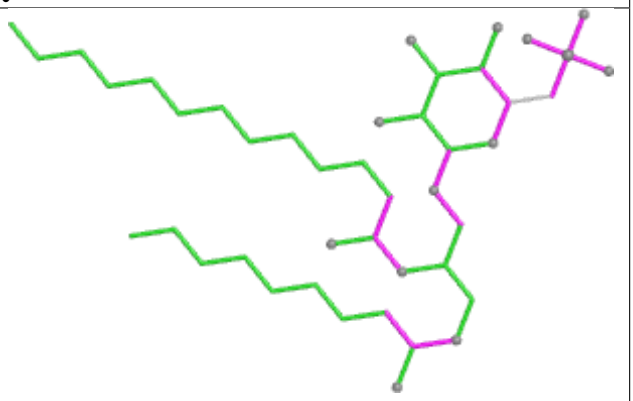


Rings

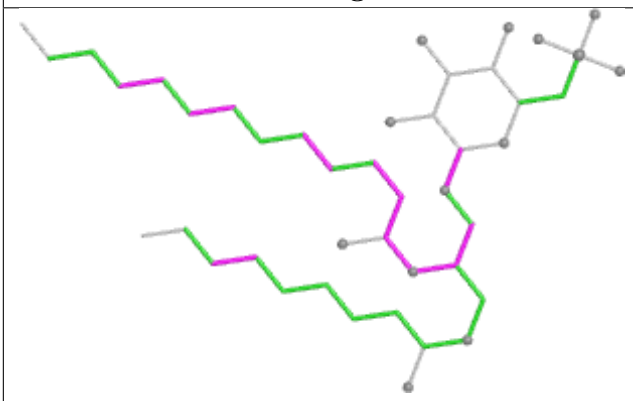
Ligand SQD d 409



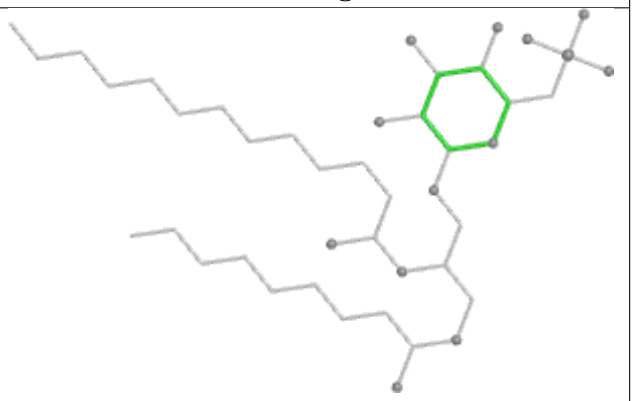
Bond lengths



Bond angles

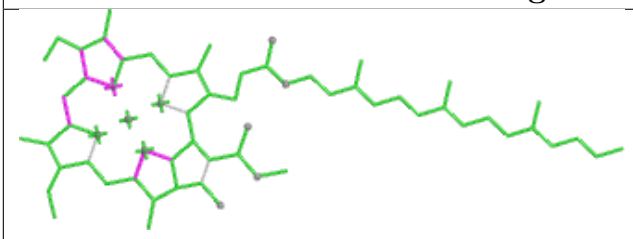


Torsions

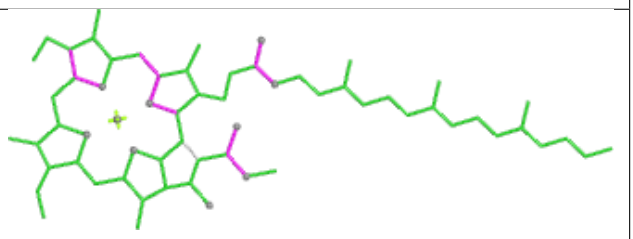


Rings

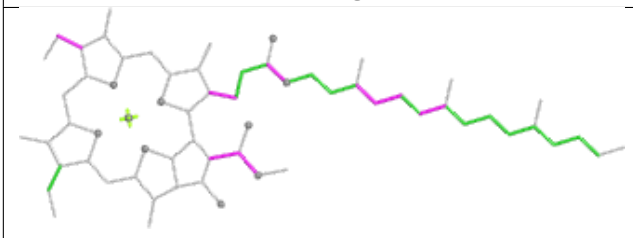
Ligand CLA 9 314



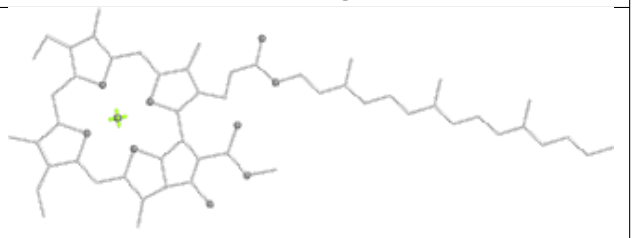
Bond lengths



Bond angles

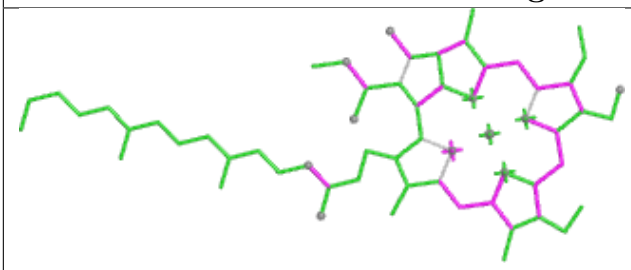


Torsions

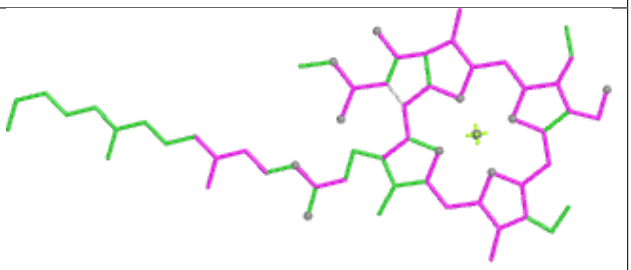


Rings

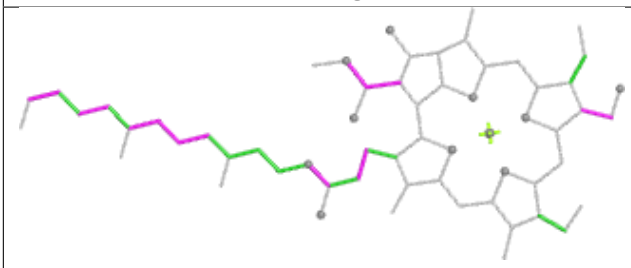
Ligand CHL 8 304



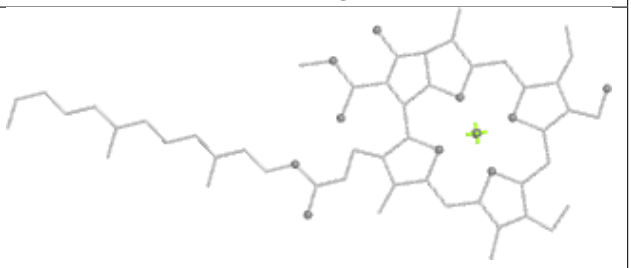
Bond lengths



Bond angles

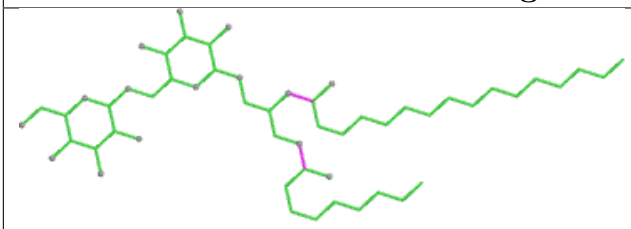


Torsions

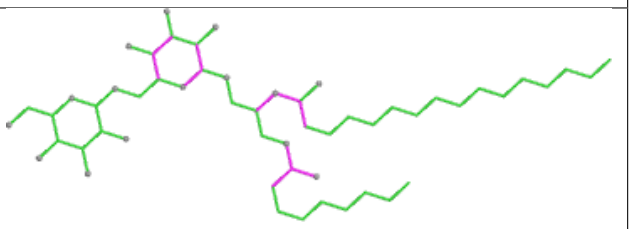


Rings

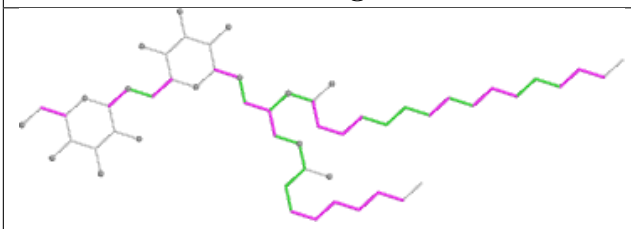
Ligand DGD C 620



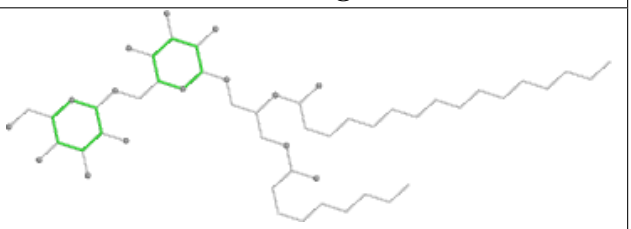
Bond lengths



Bond angles

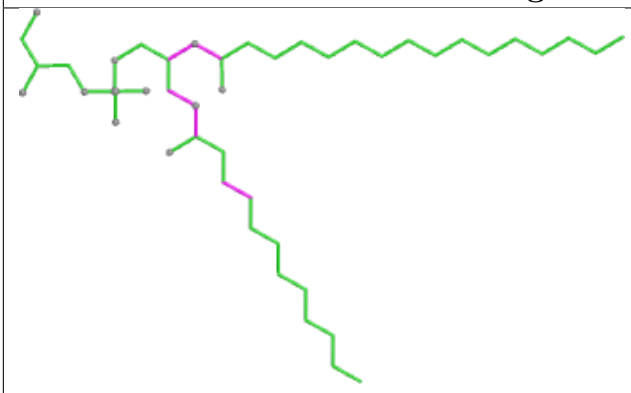


Torsions

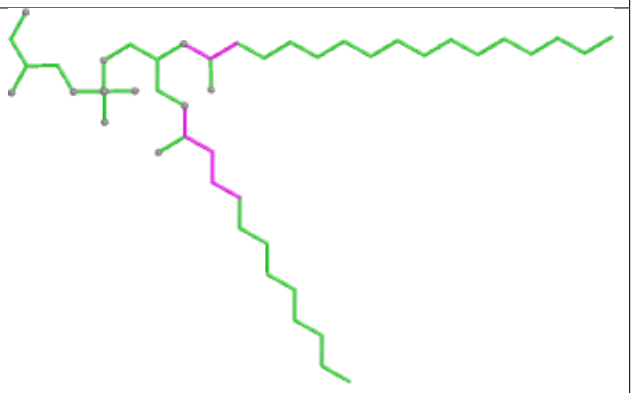


Rings

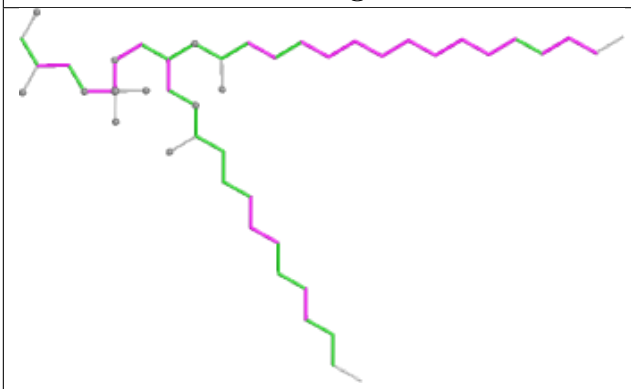
Ligand LHG a 601



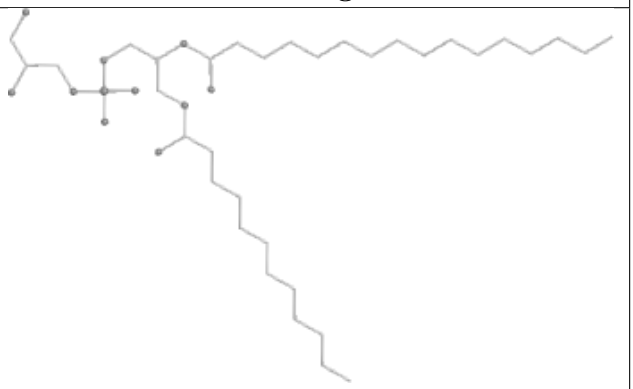
Bond lengths



Bond angles

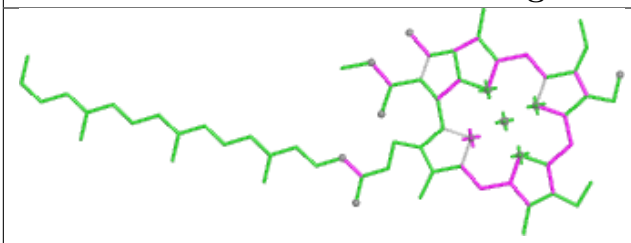


Torsions

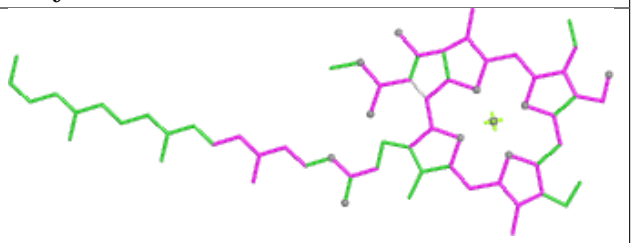


Rings

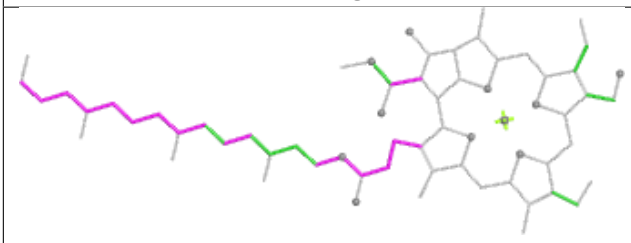
Ligand CHL y 306



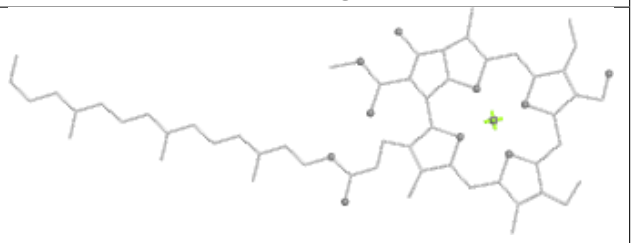
Bond lengths



Bond angles

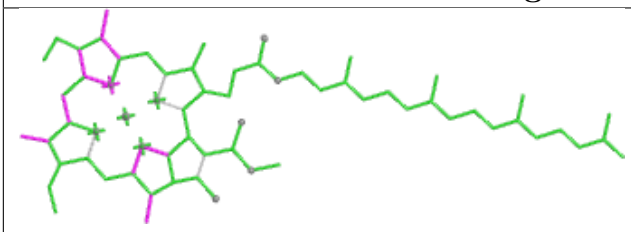


Torsions

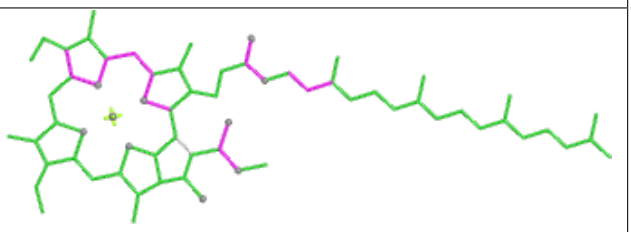


Rings

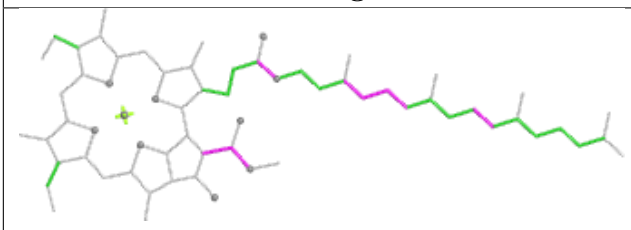
Ligand CLA B 613



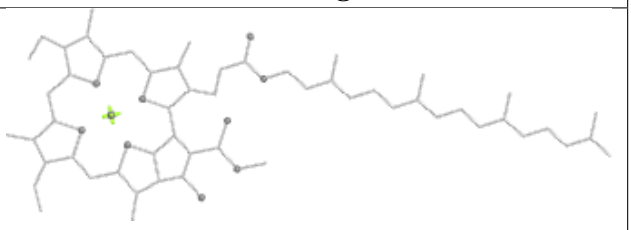
Bond lengths



Bond angles

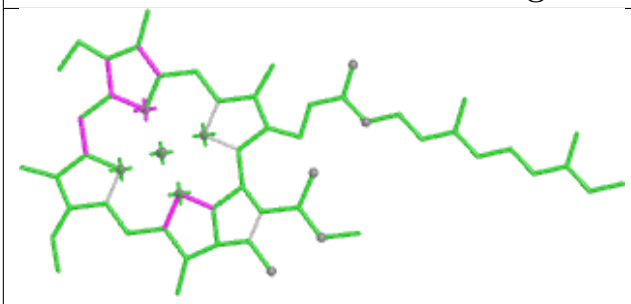


Torsions

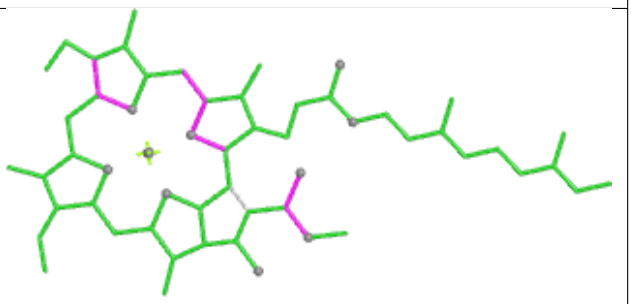


Rings

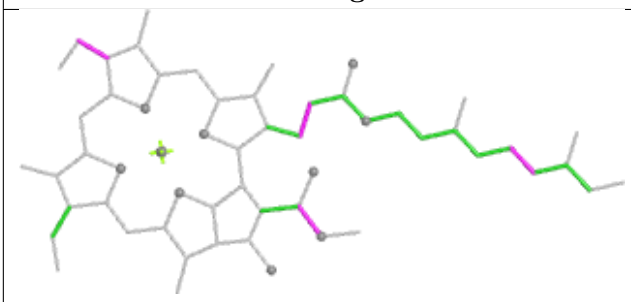
Ligand CLA u 307



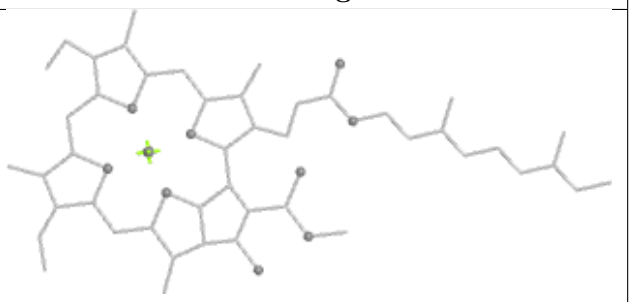
Bond lengths



Bond angles

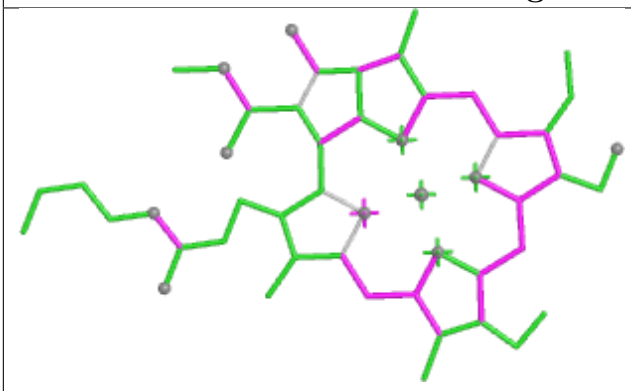


Torsions

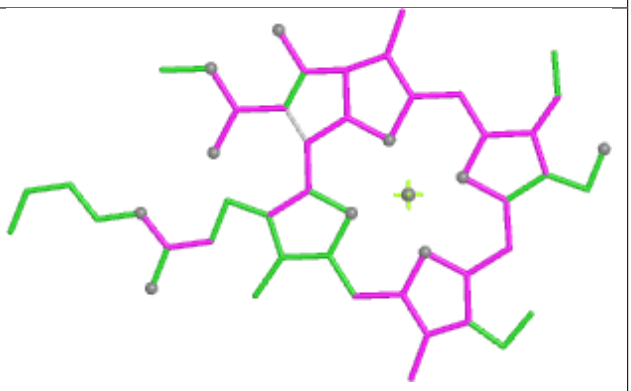


Rings

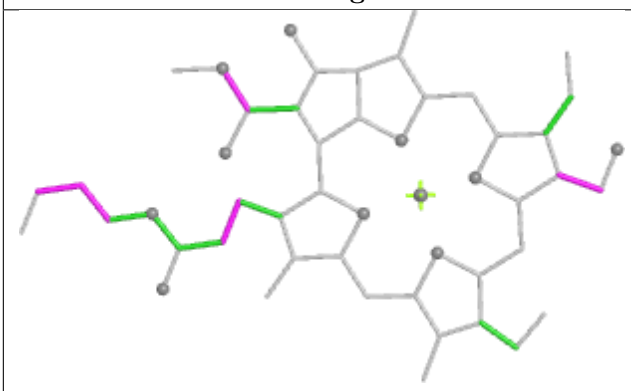
Ligand CHL n 311



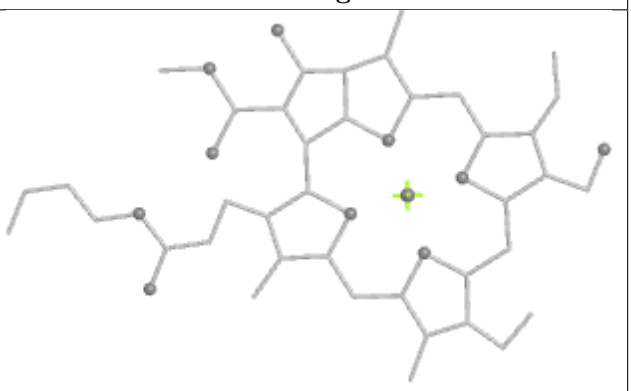
Bond lengths



Bond angles

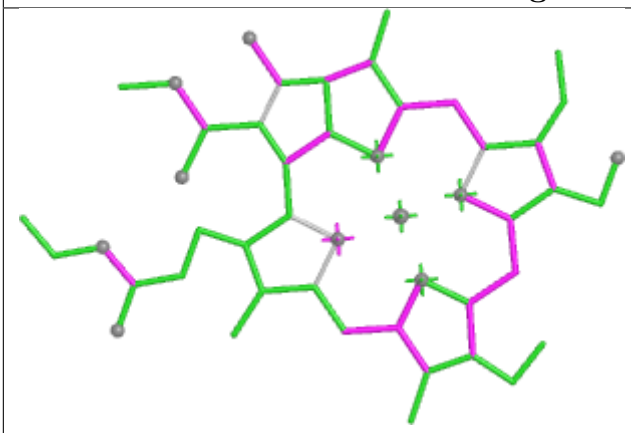


Torsions

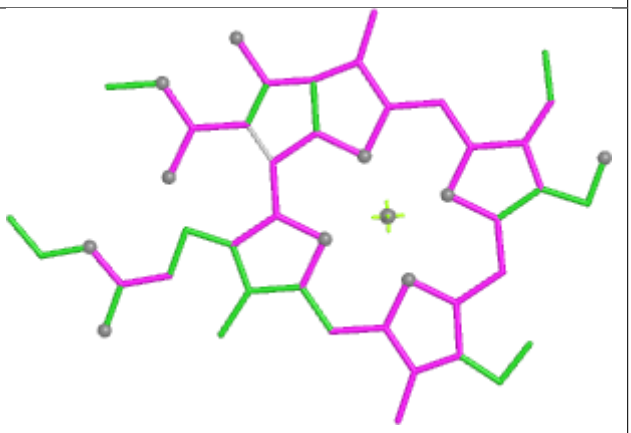


Rings

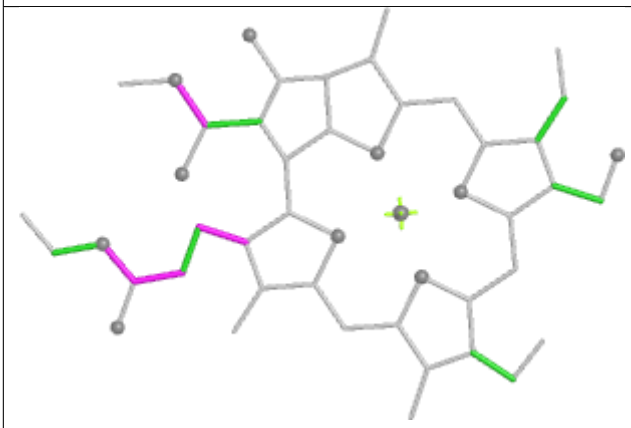
Ligand CHL r 307



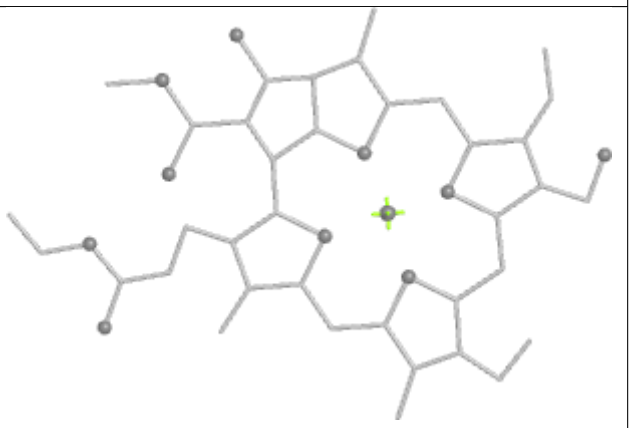
Bond lengths



Bond angles

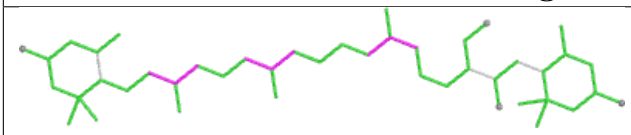


Torsions

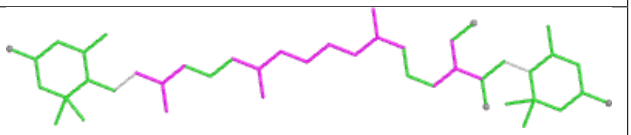


Rings

Ligand 0IE 8 302



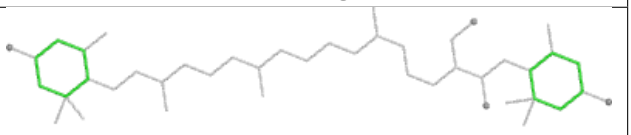
Bond lengths



Bond angles

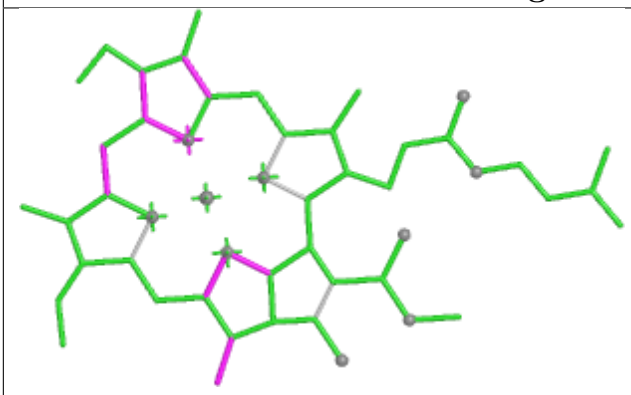


Torsions

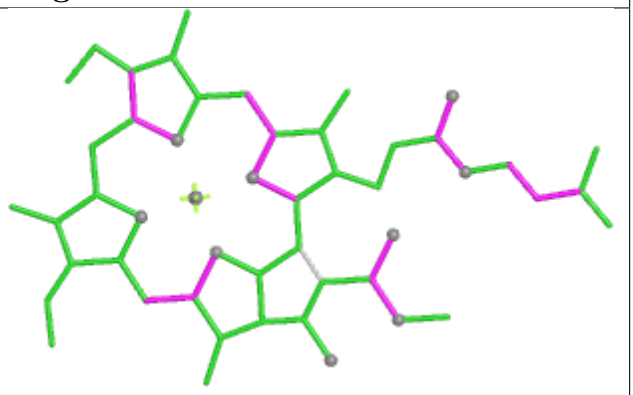


Rings

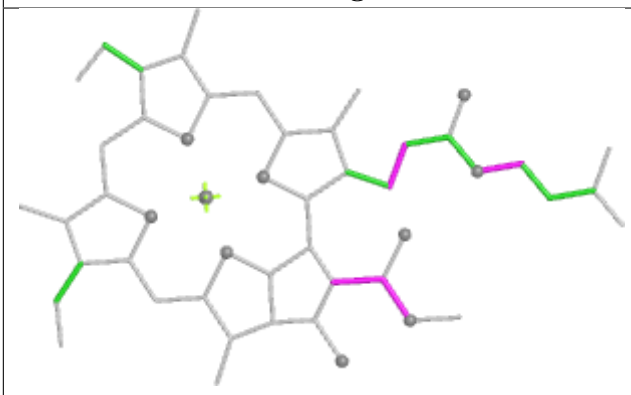
Ligand CLA g 308



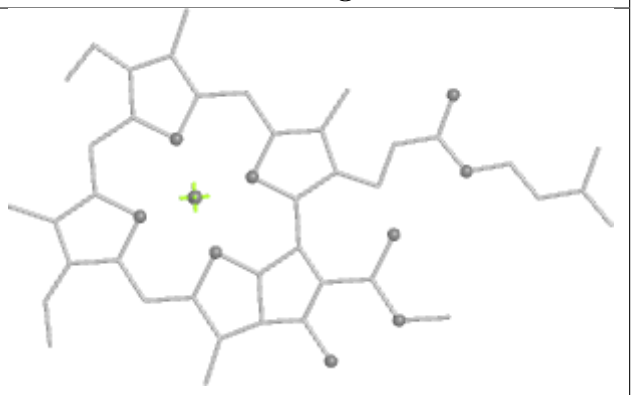
Bond lengths



Bond angles

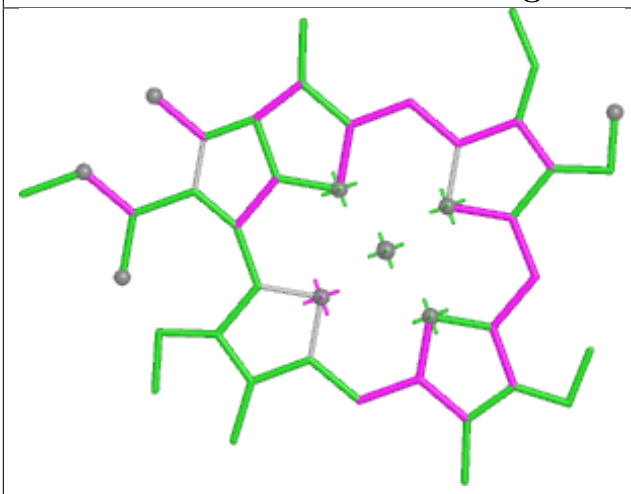


Torsions

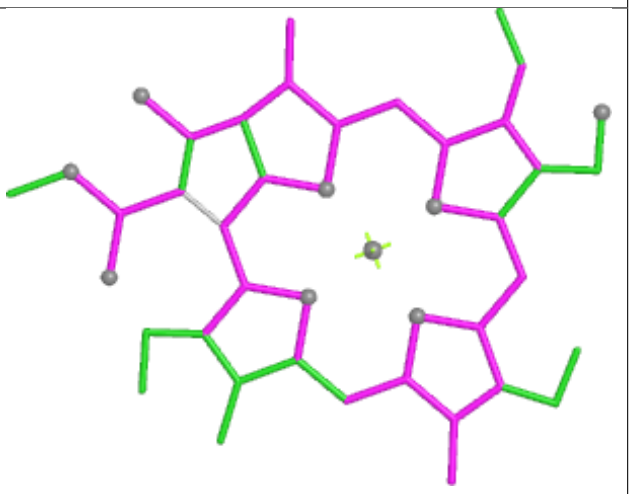


Rings

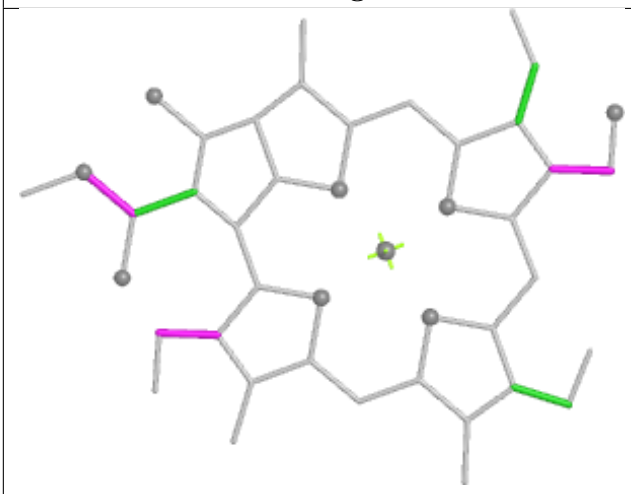
Ligand CHL Y 308



Bond lengths



Bond angles

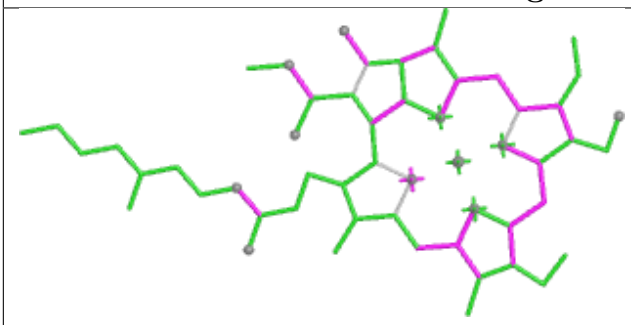


Torsions

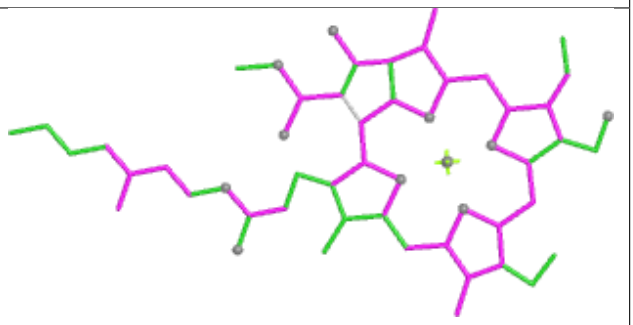


Rings

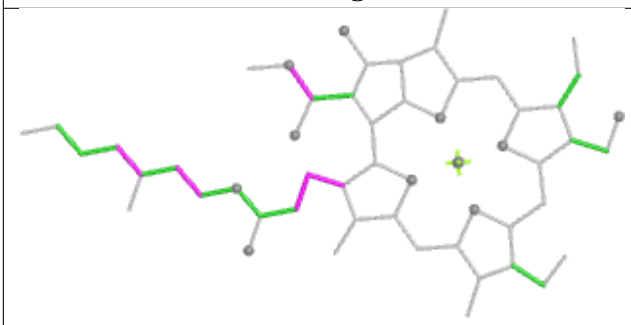
Ligand CHL n 304



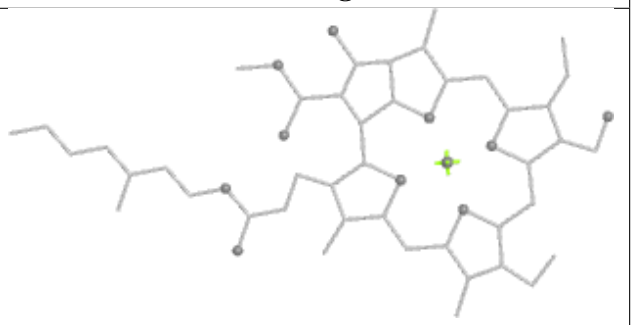
Bond lengths



Bond angles

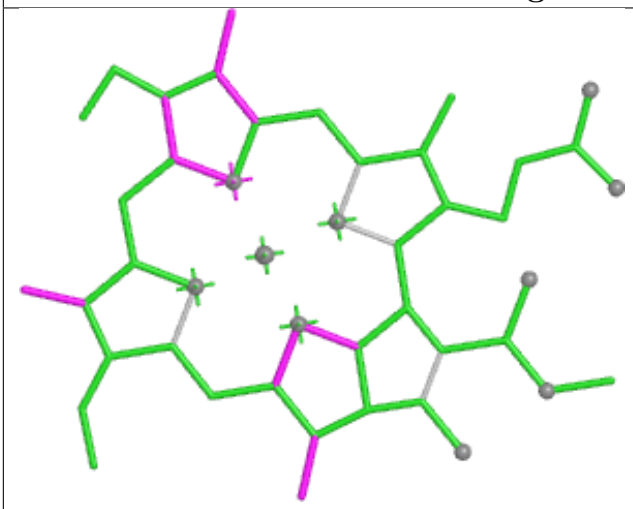


Torsions

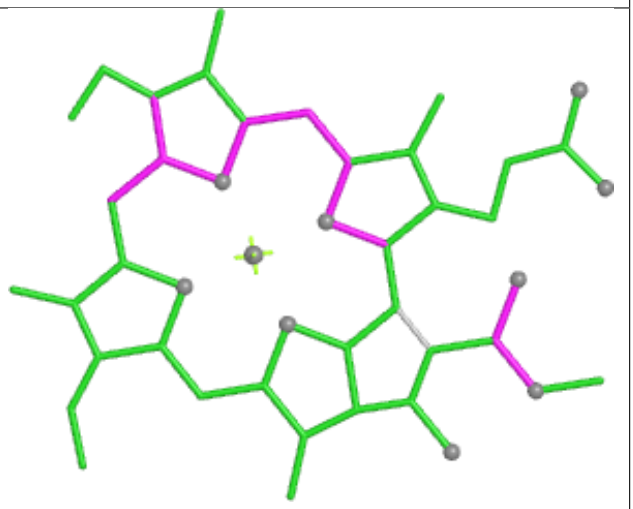


Rings

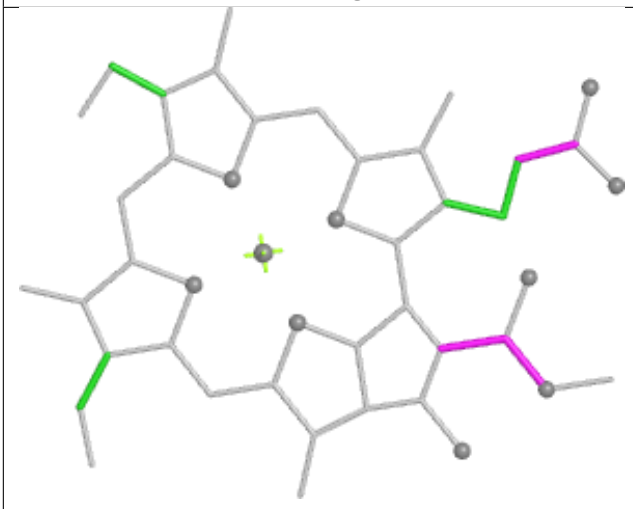
Ligand CLA S 603



Bond lengths



Bond angles

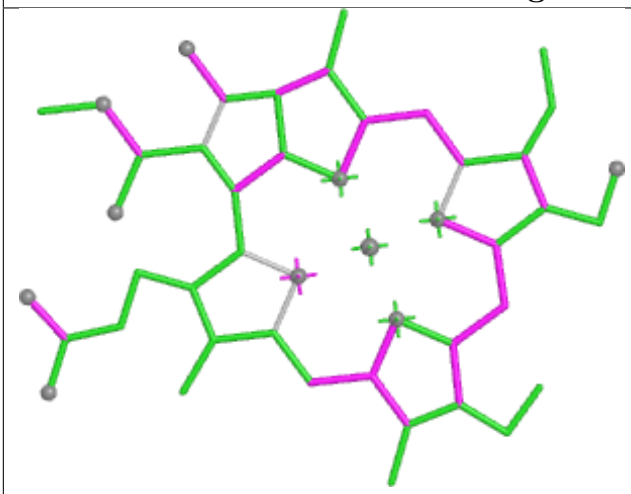


Torsions

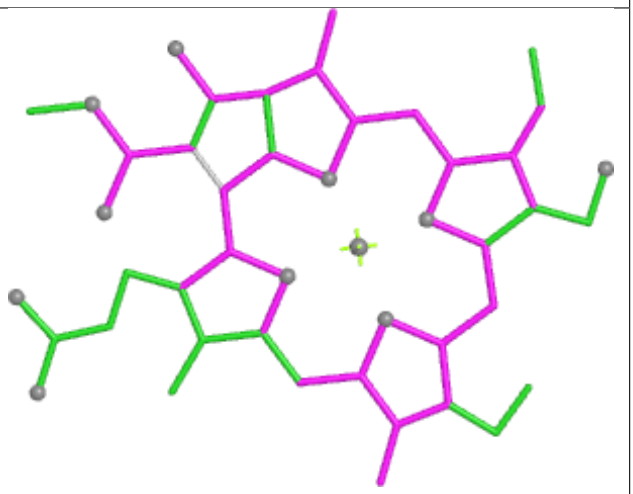


Rings

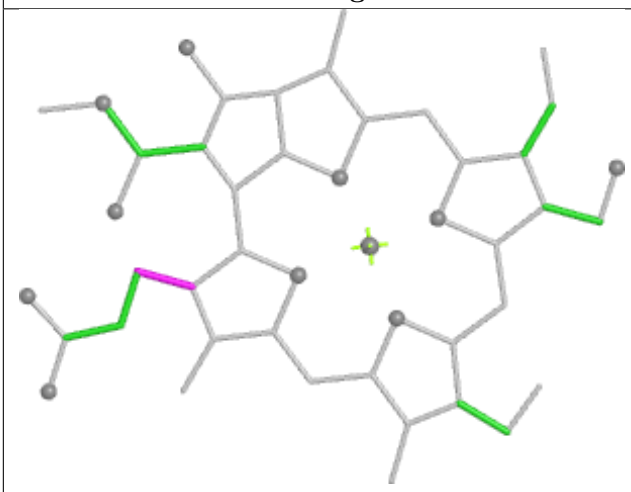
Ligand CHL 7 311



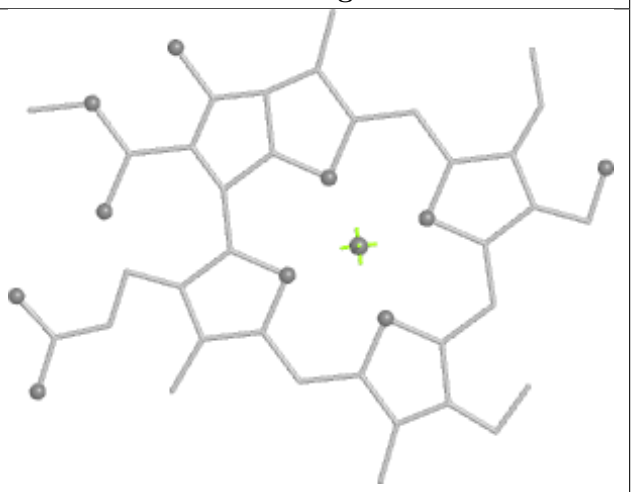
Bond lengths



Bond angles

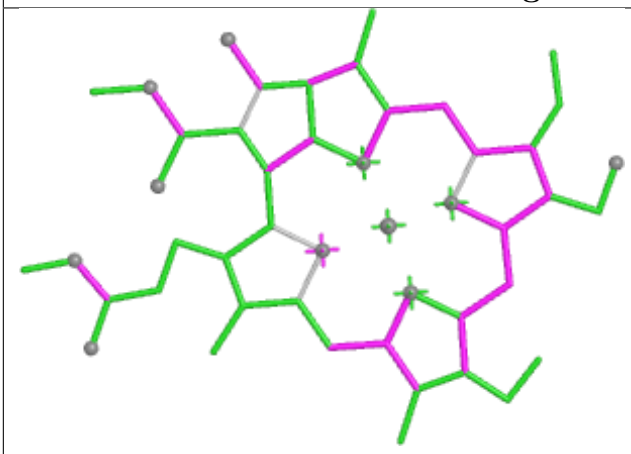


Torsions

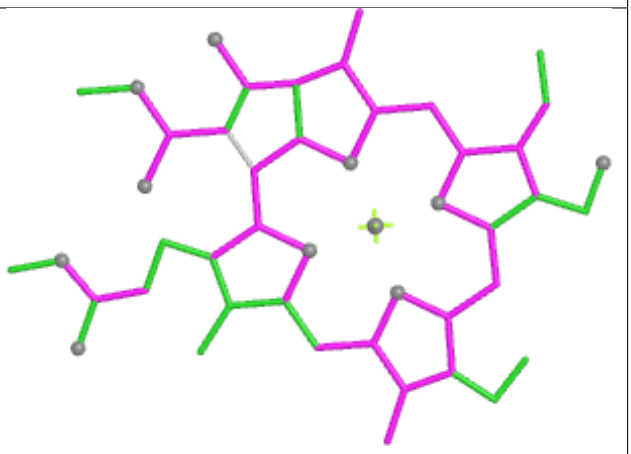


Rings

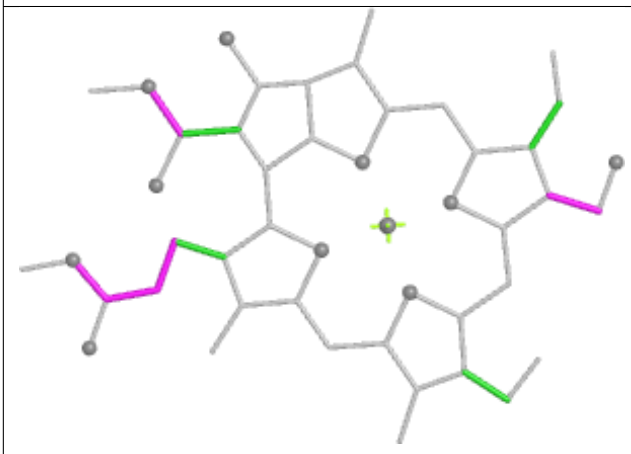
Ligand CHL G 310



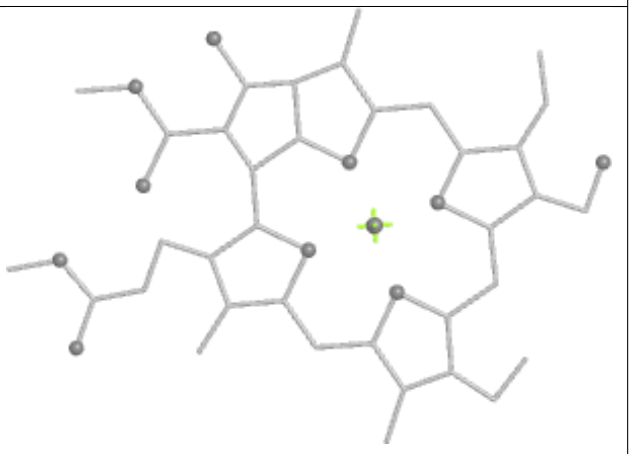
Bond lengths



Bond angles

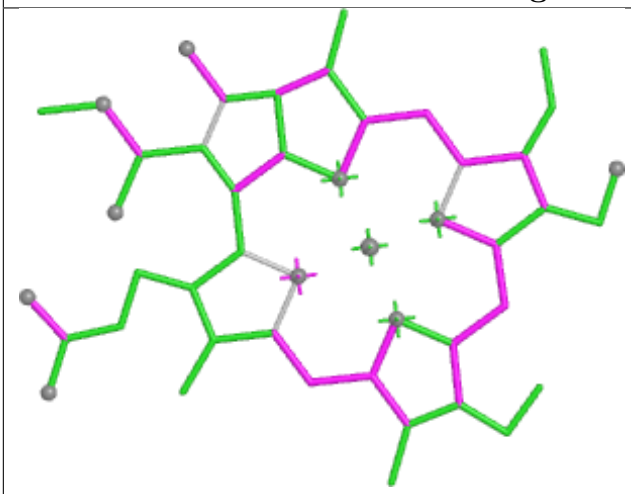


Torsions

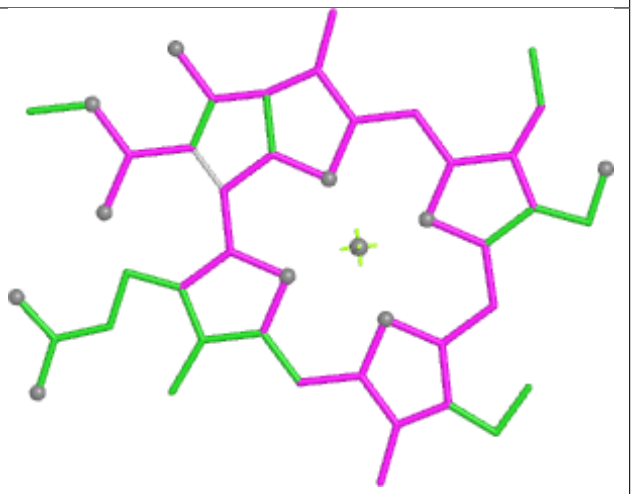


Rings

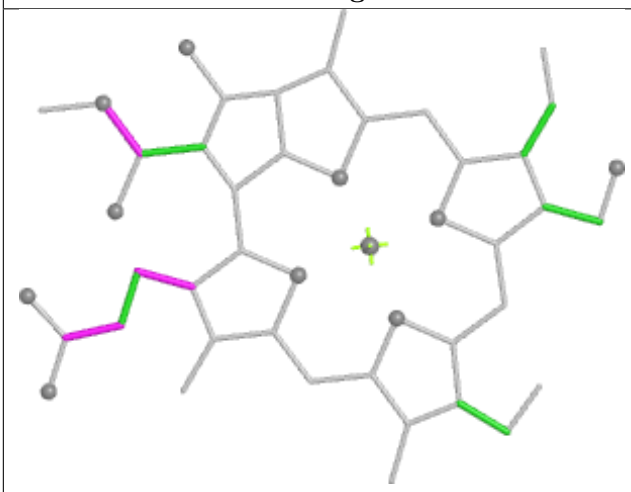
Ligand CHL s 407



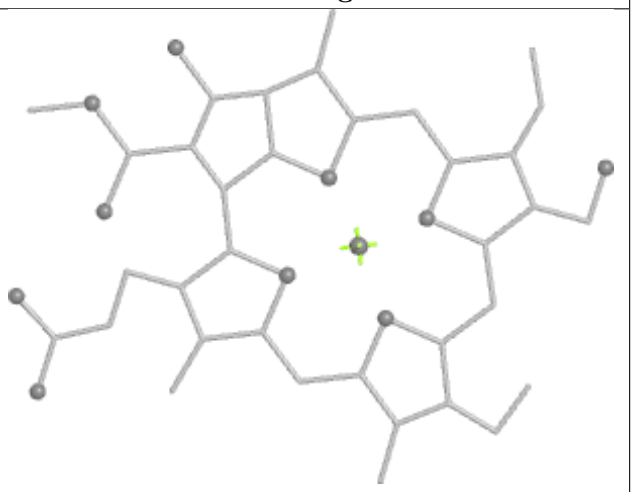
Bond lengths



Bond angles

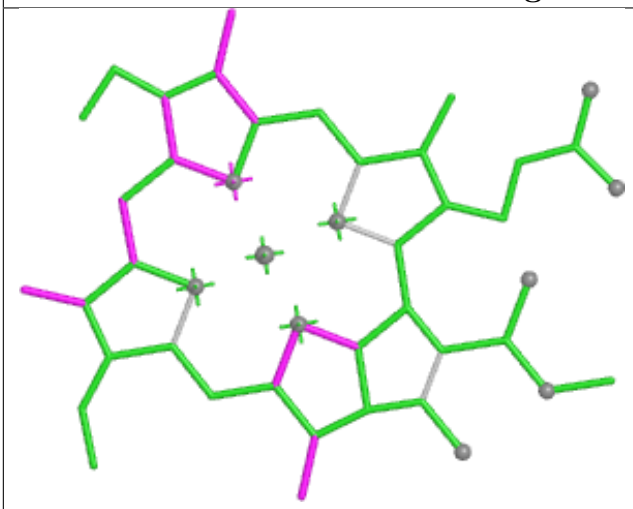


Torsions

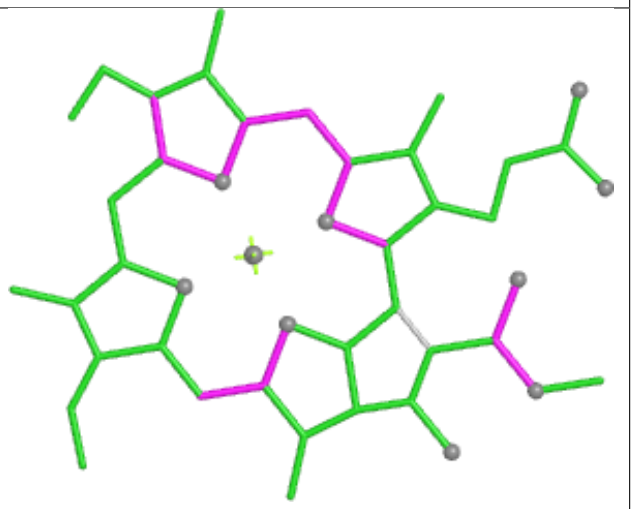


Rings

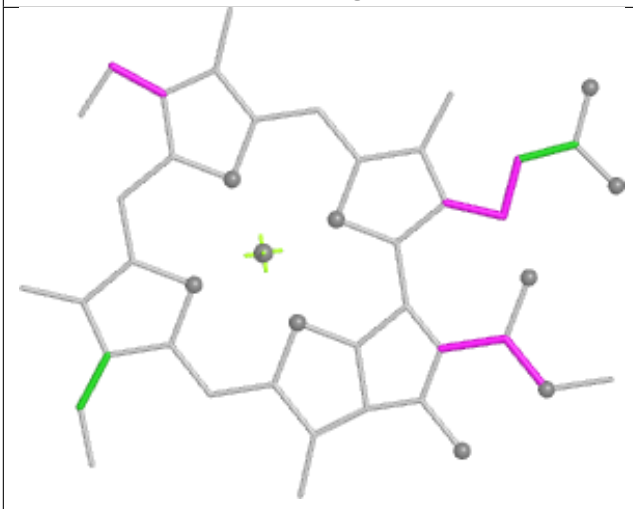
Ligand CLA B 601



Bond lengths



Bond angles

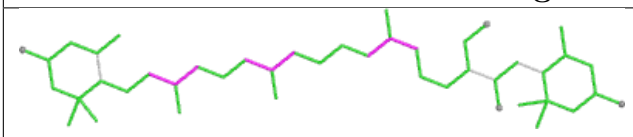


Torsions

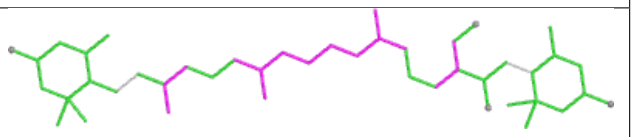


Rings

Ligand 0IE Y 303



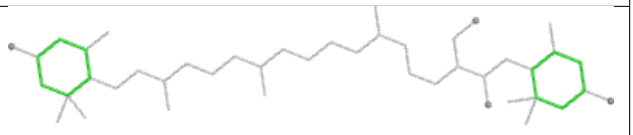
Bond lengths



Bond angles

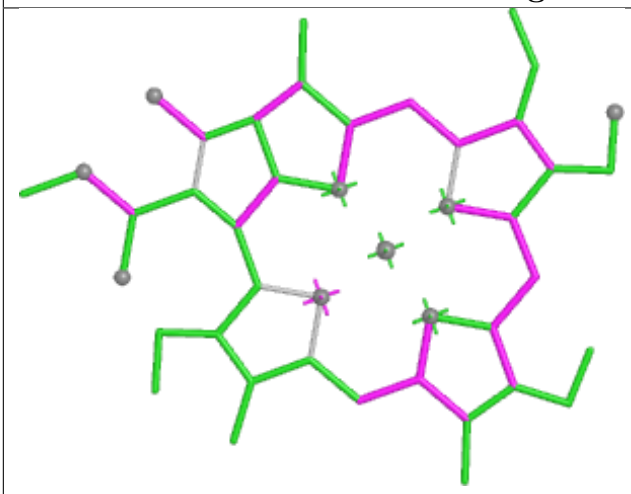


Torsions

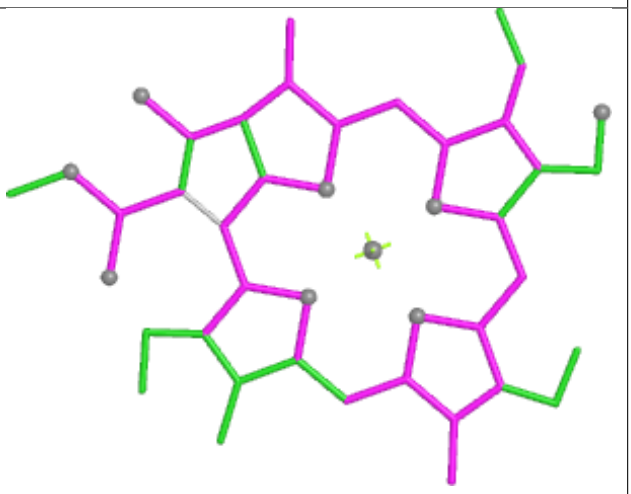


Rings

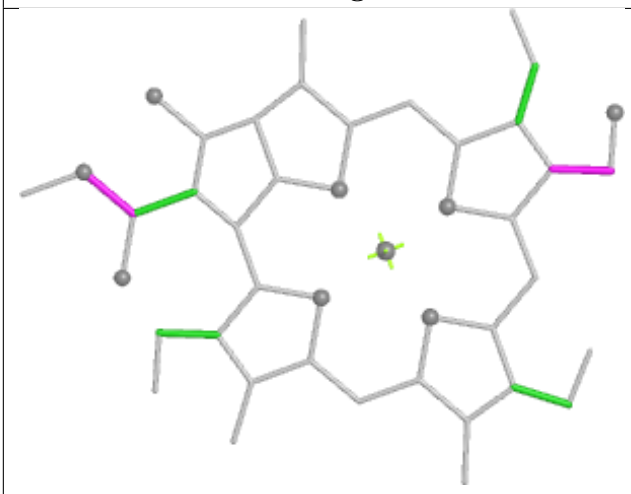
Ligand CHL 6 312



Bond lengths



Bond angles

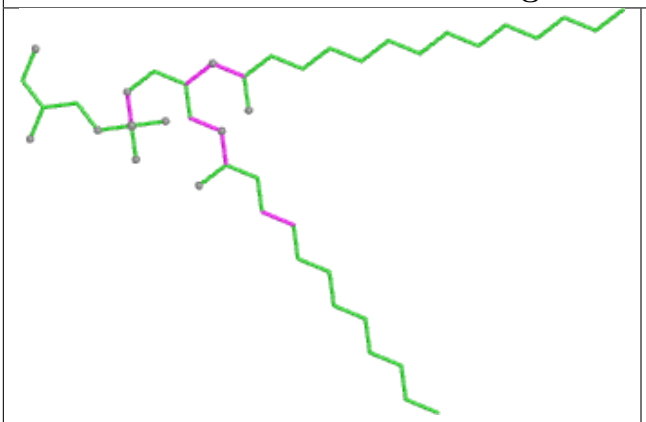


Torsions

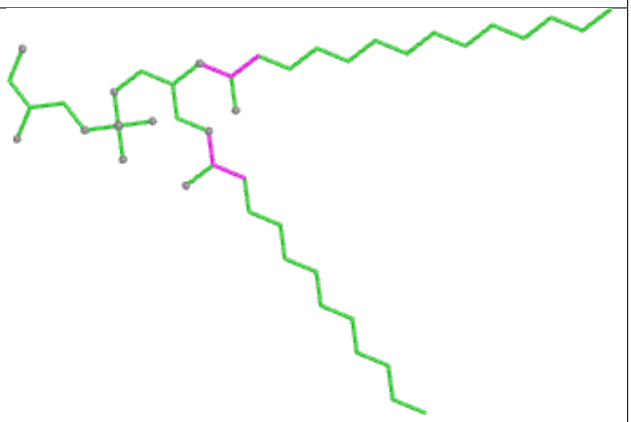


Rings

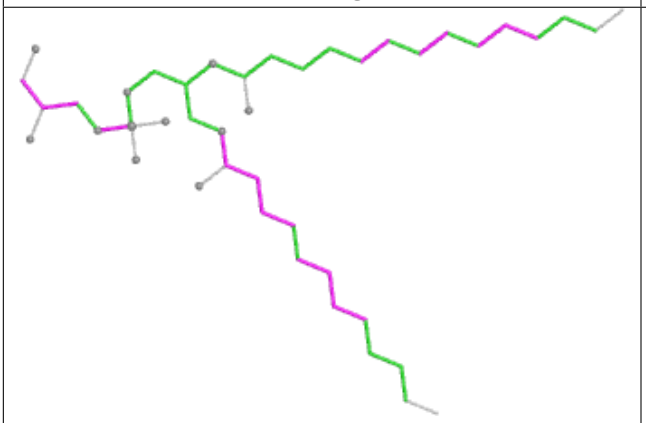
Ligand LHG N 318



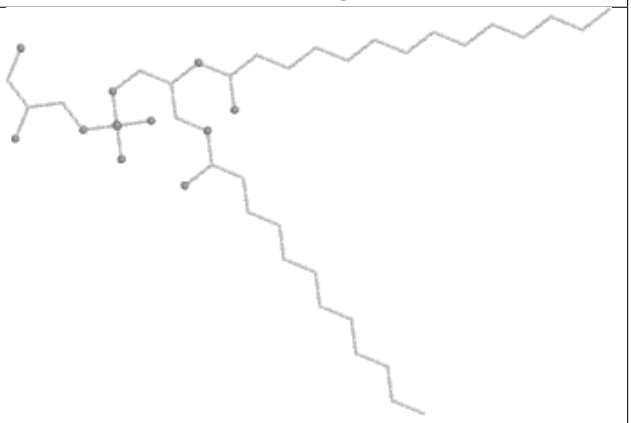
Bond lengths



Bond angles

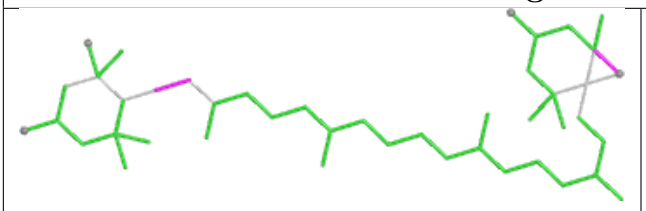


Torsions

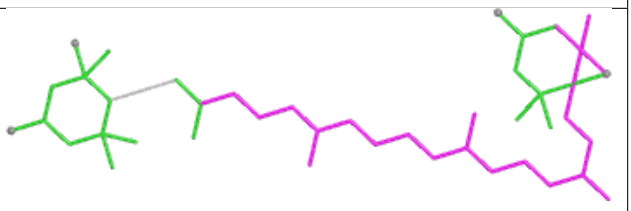


Rings

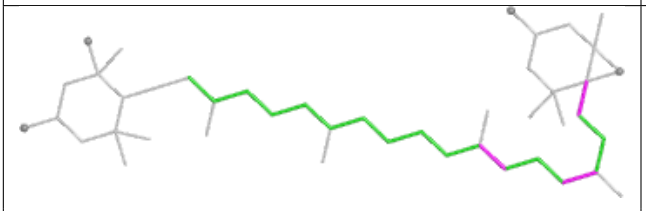
Ligand NEX 9 319



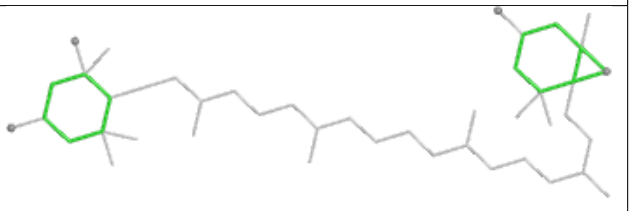
Bond lengths



Bond angles

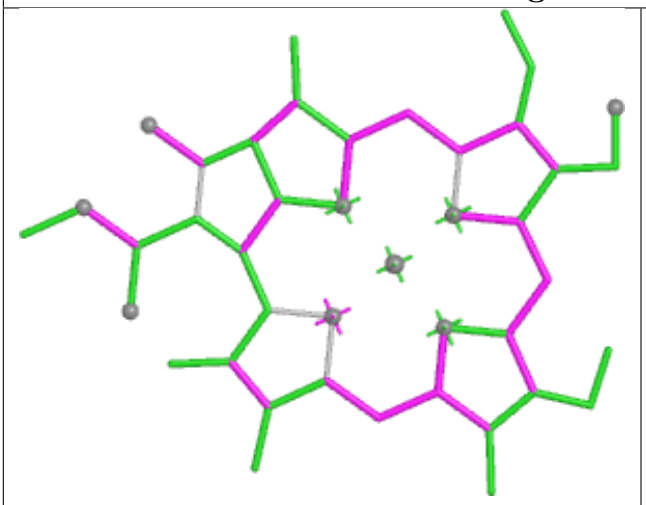


Torsions

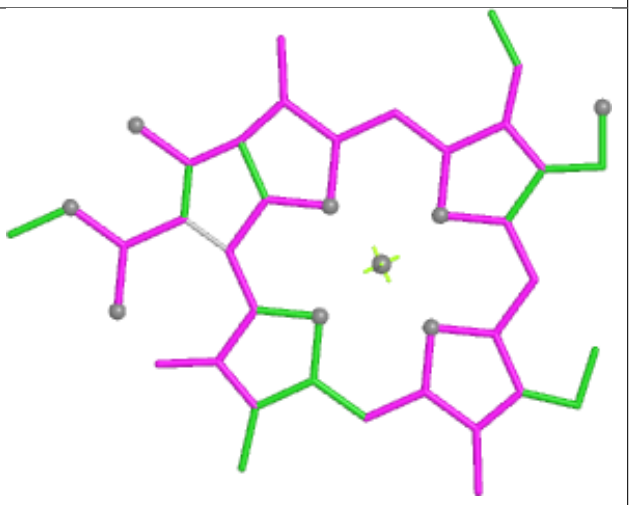


Rings

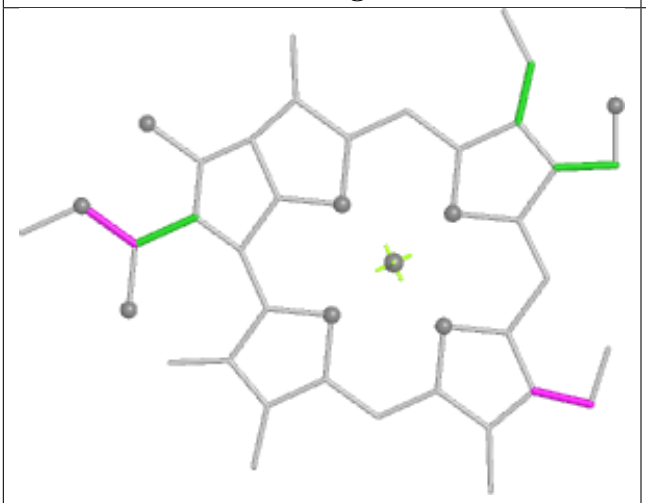
Ligand CHL 5 310



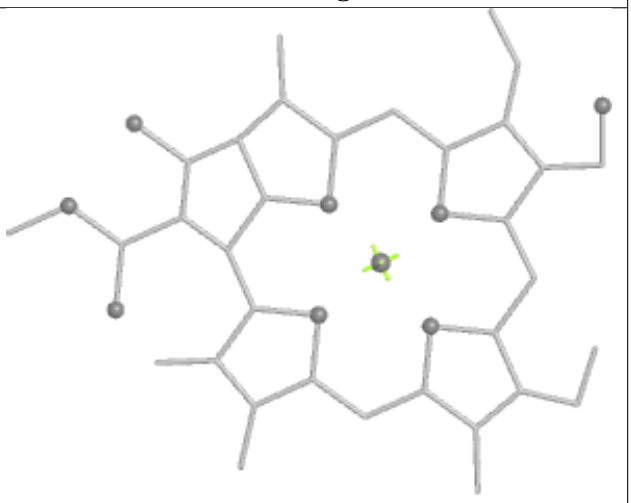
Bond lengths



Bond angles

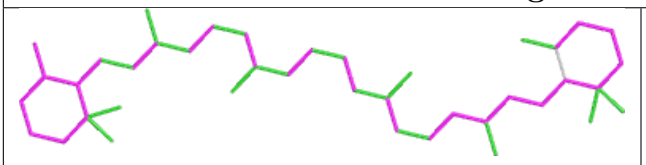


Torsions

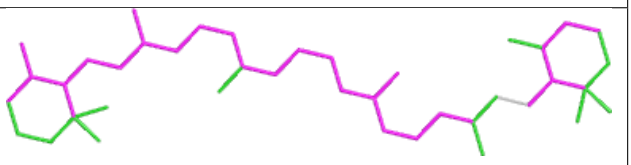


Rings

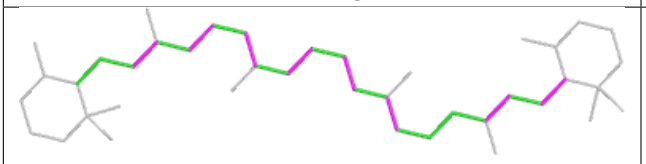
Ligand 8CT B 617



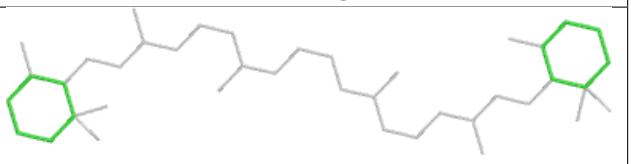
Bond lengths



Bond angles

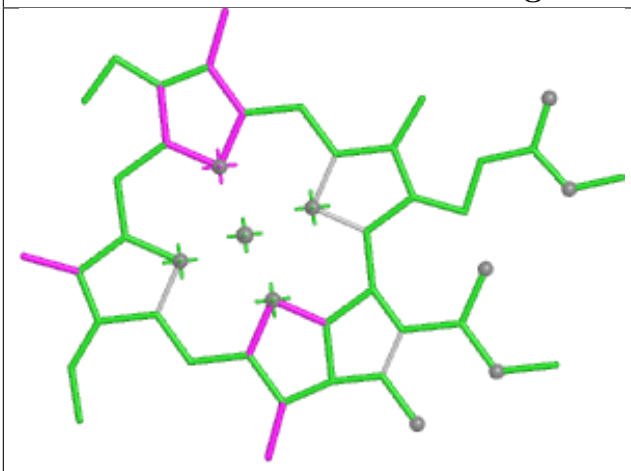


Torsions

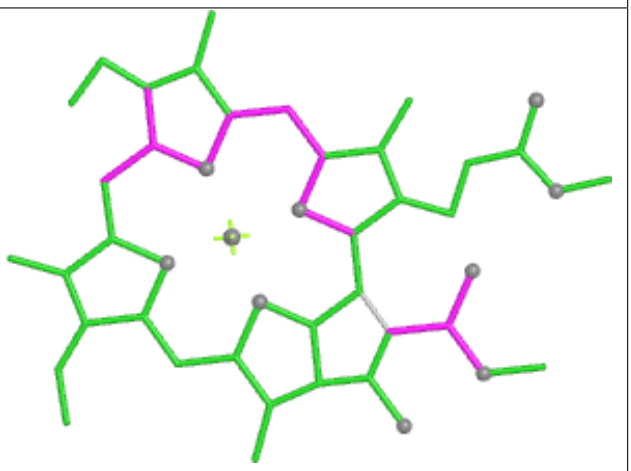


Rings

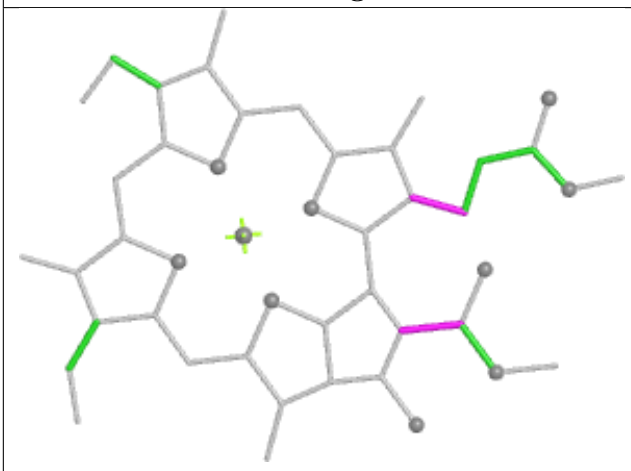
Ligand CLA C 616



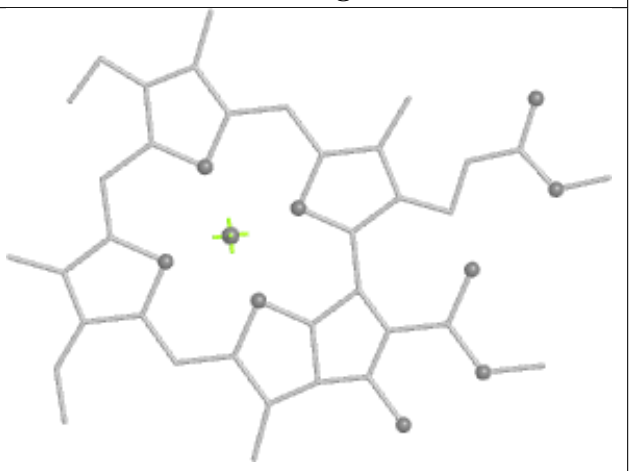
Bond lengths



Bond angles

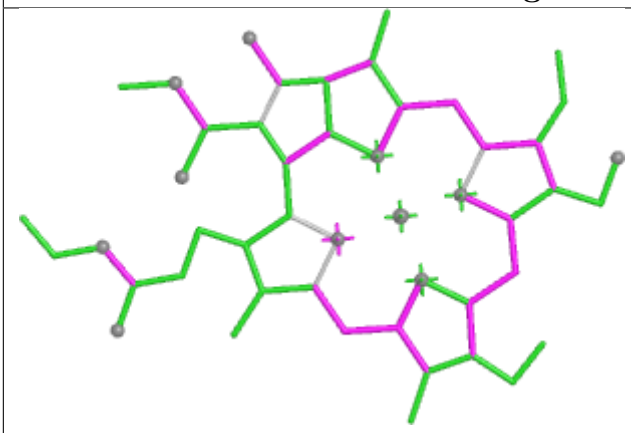


Torsions

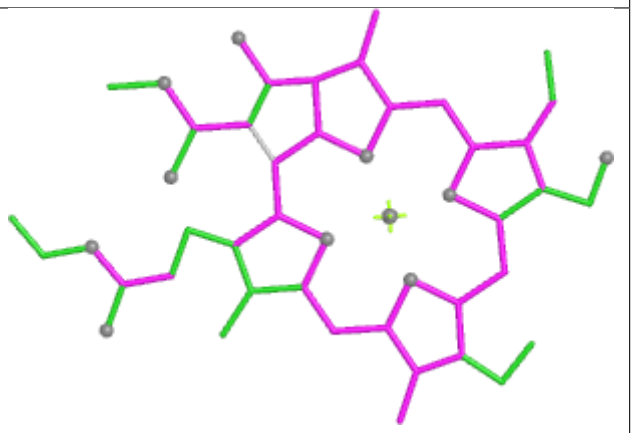


Rings

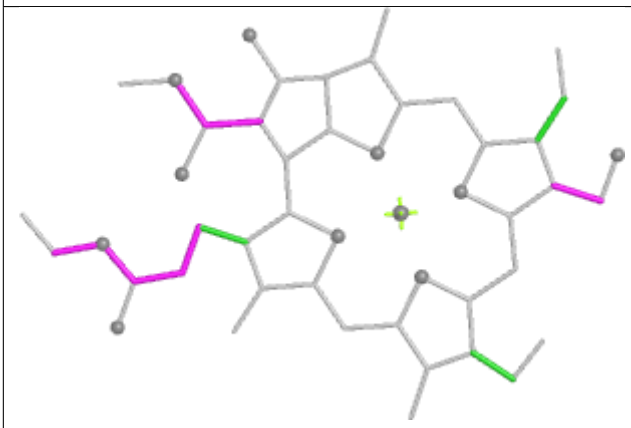
Ligand CHL R 607



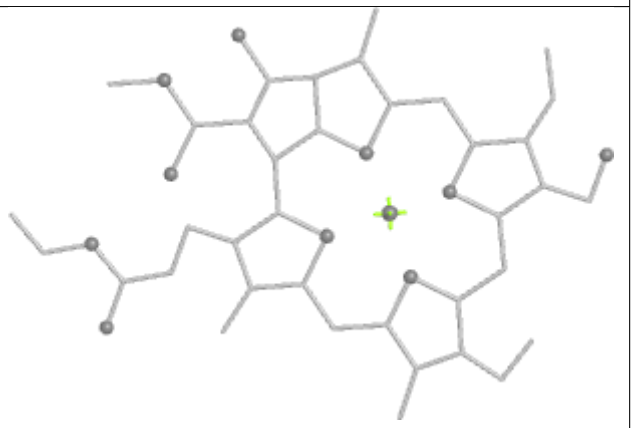
Bond lengths



Bond angles

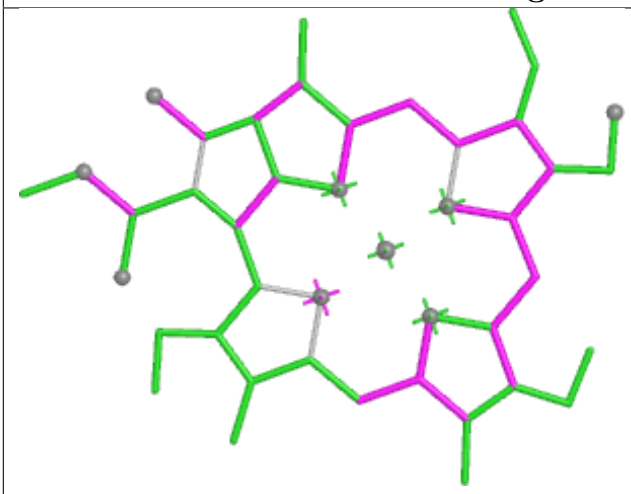


Torsions

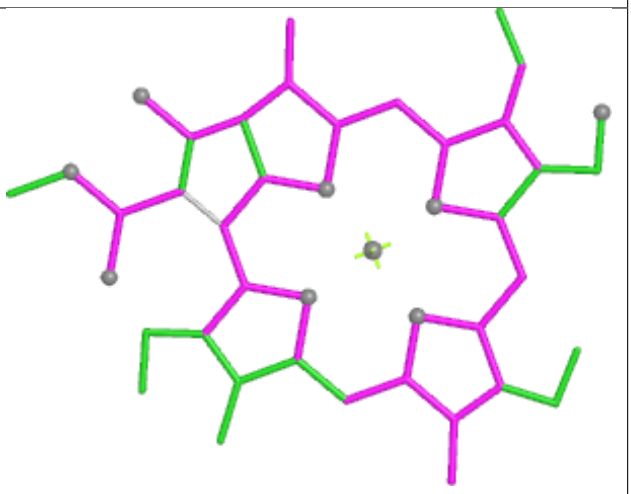


Rings

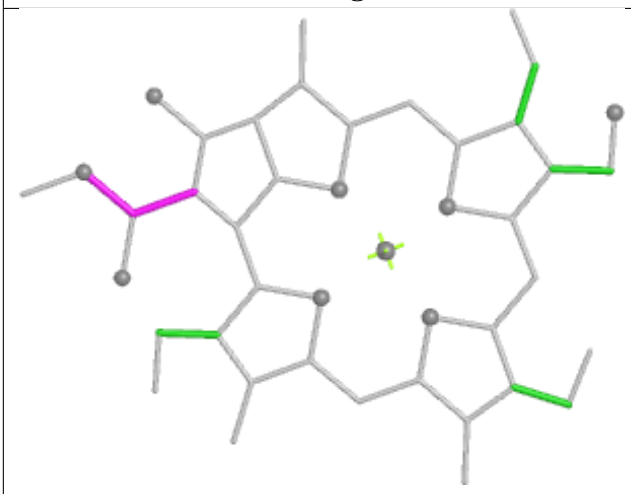
Ligand CHL 2 309



Bond lengths



Bond angles

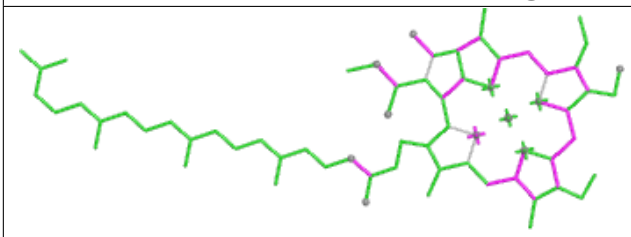


Torsions

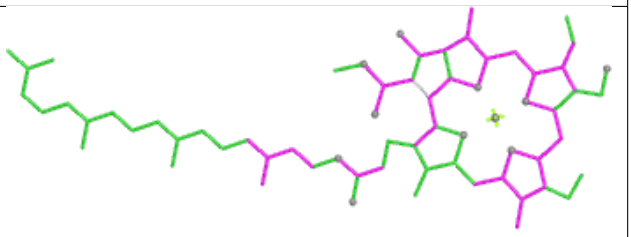


Rings

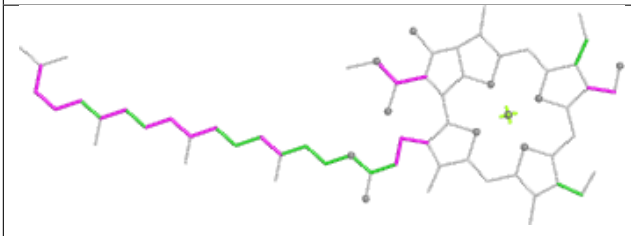
Ligand CHL G 305



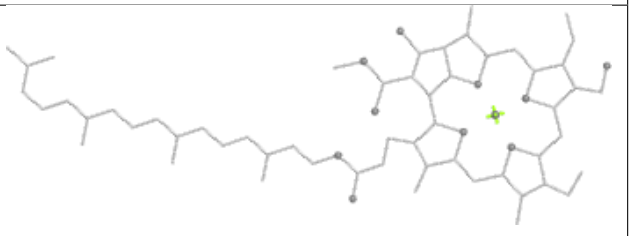
Bond lengths



Bond angles

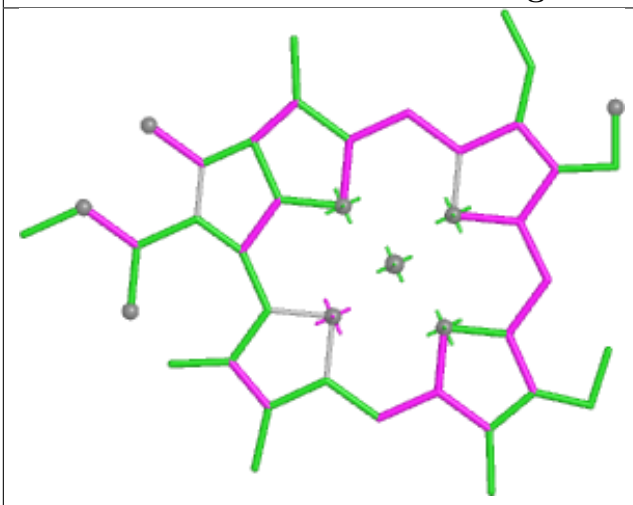


Torsions

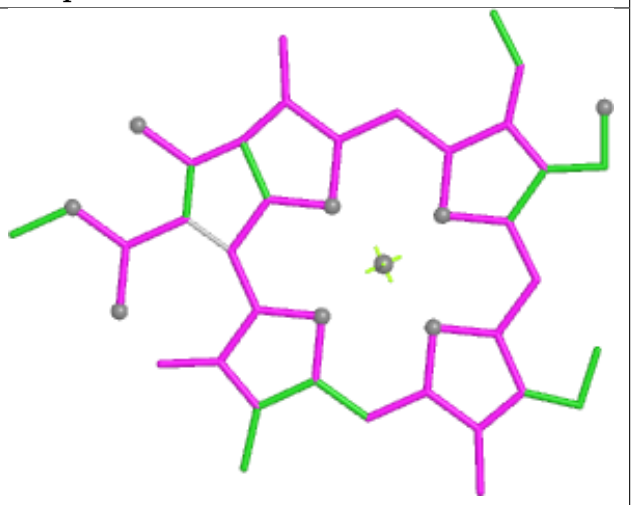


Rings

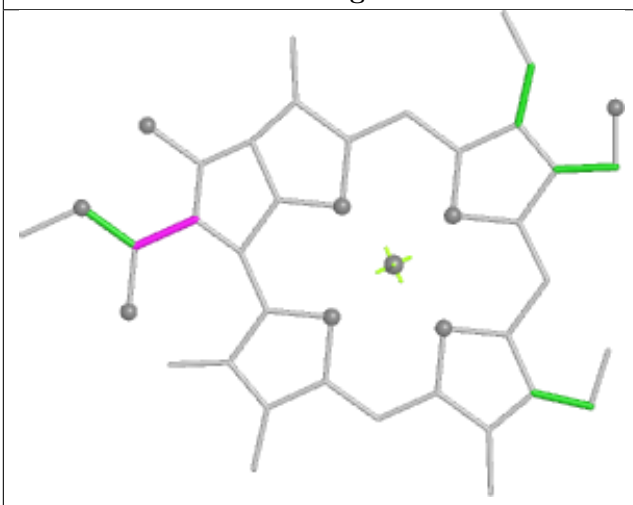
Ligand CHL q 316



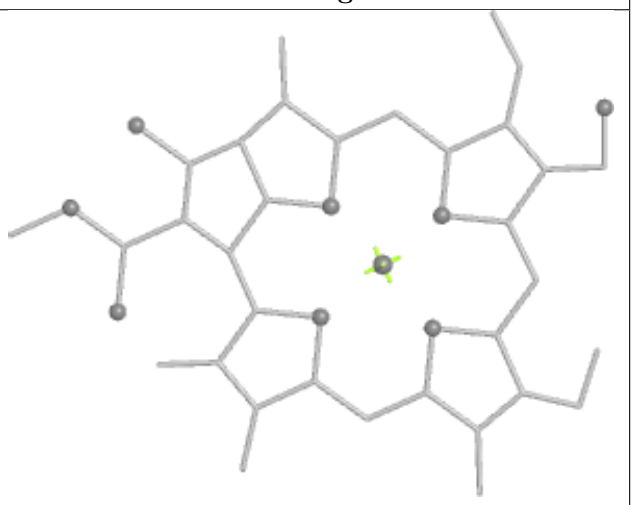
Bond lengths



Bond angles

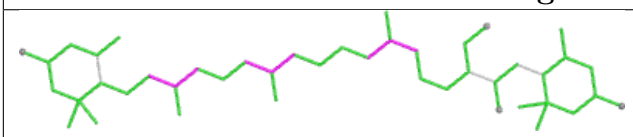


Torsions

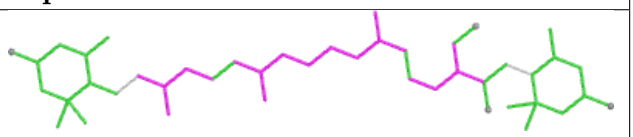


Rings

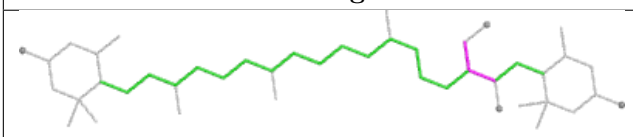
Ligand 0IE p 302



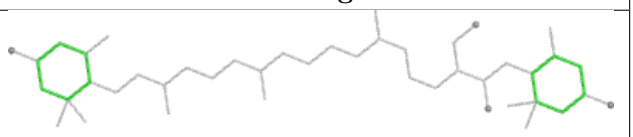
Bond lengths



Bond angles

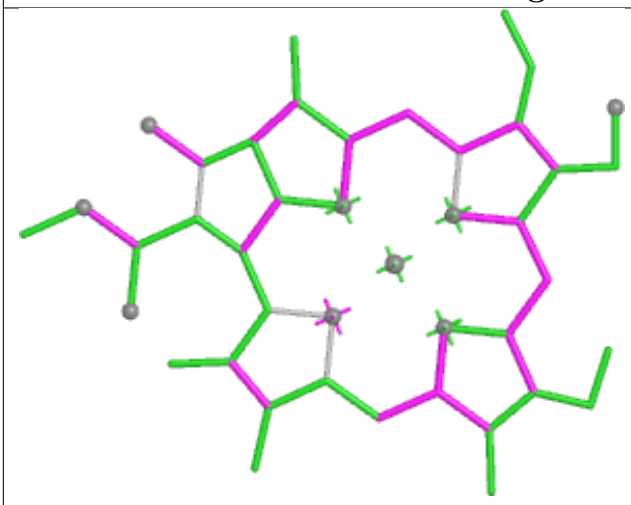


Torsions

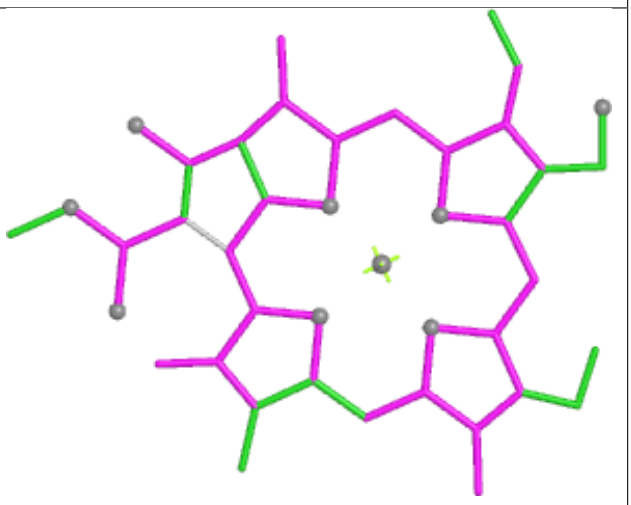


Rings

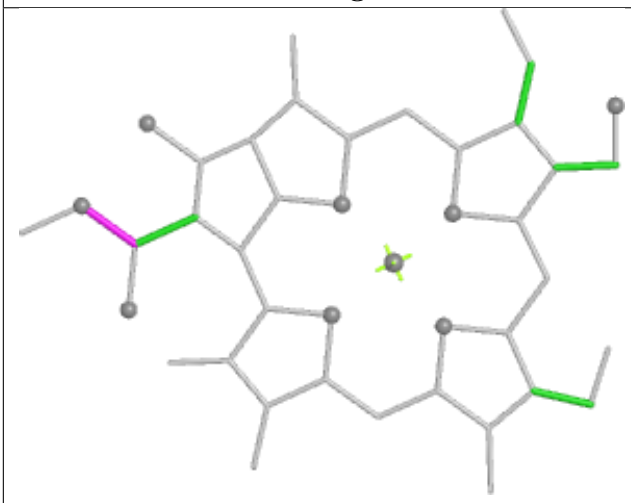
Ligand CHL 1 304



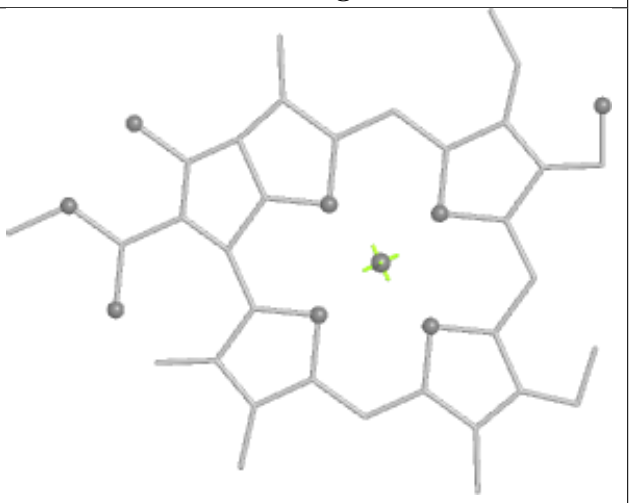
Bond lengths



Bond angles

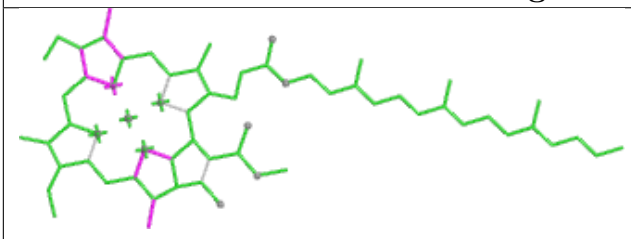


Torsions

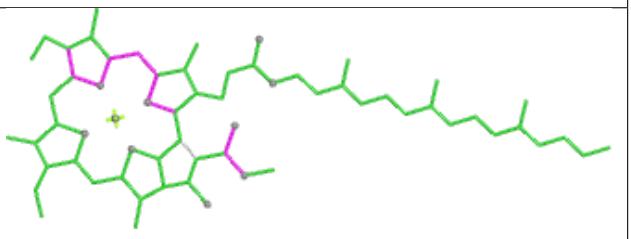


Rings

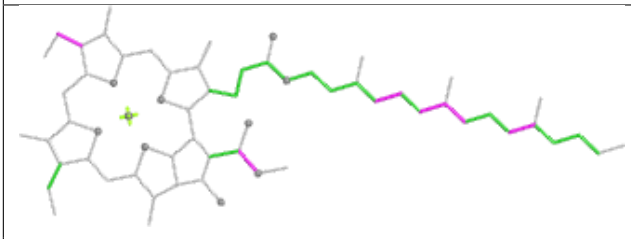
Ligand CLA 2 315



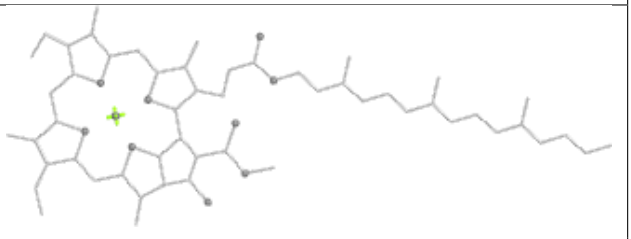
Bond lengths



Bond angles

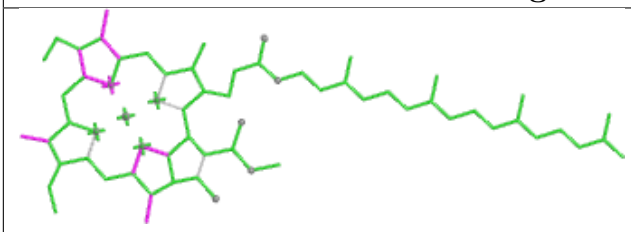


Torsions

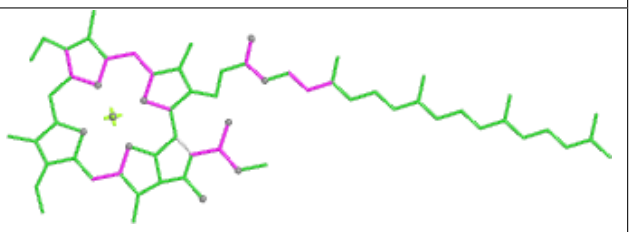


Rings

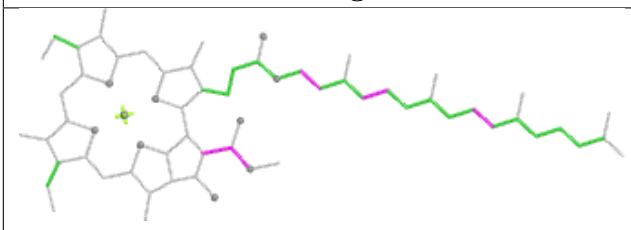
Ligand CLA c 609



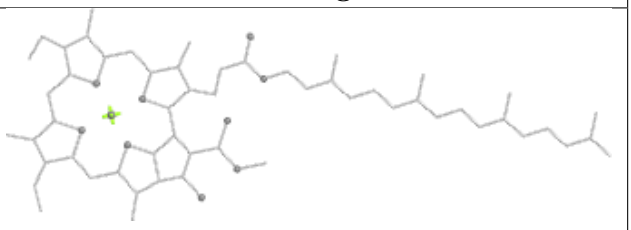
Bond lengths



Bond angles

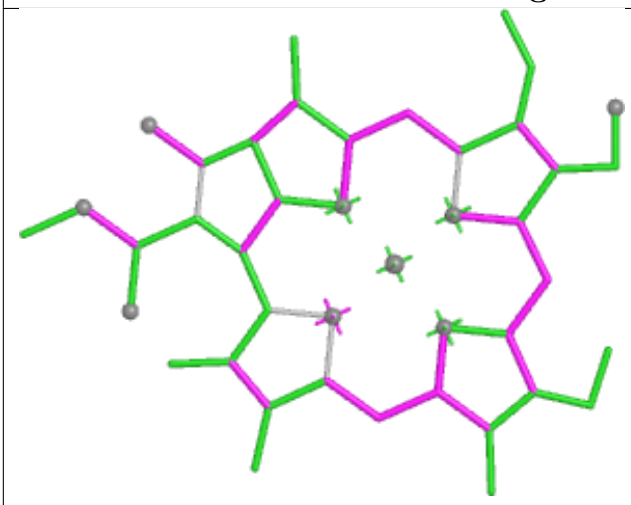


Torsions

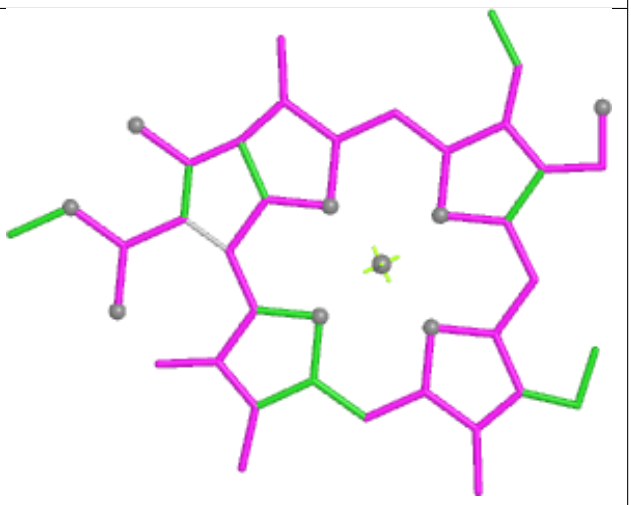


Rings

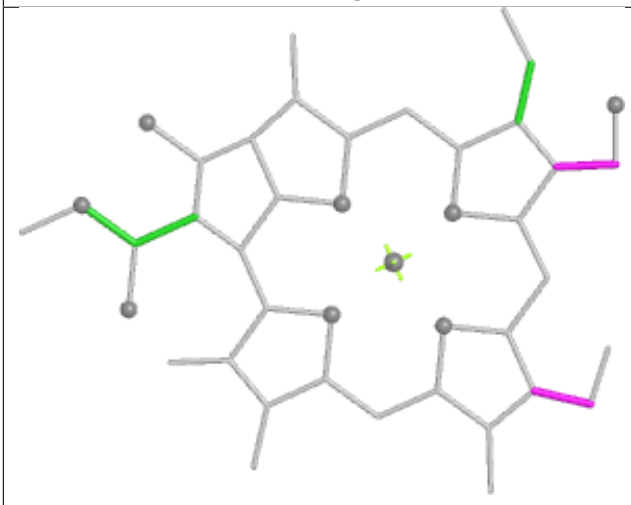
Ligand CHL s 414



Bond lengths



Bond angles

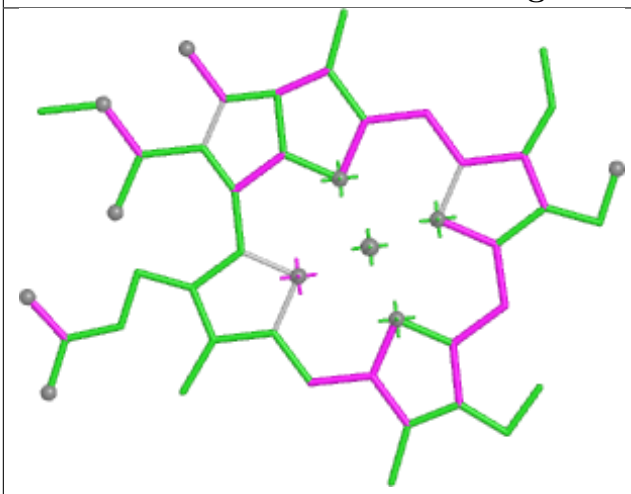


Torsions

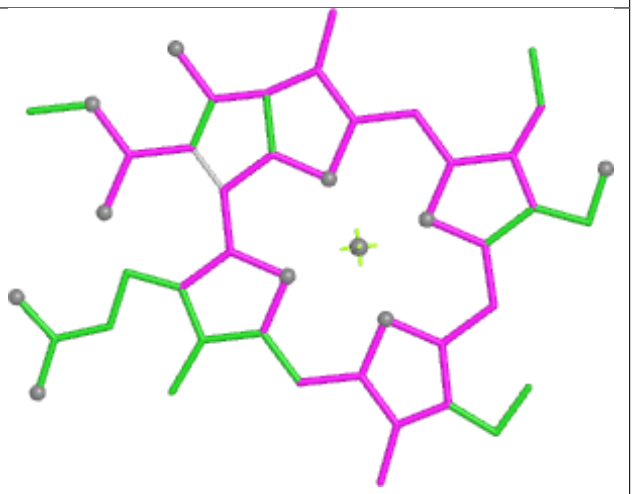


Rings

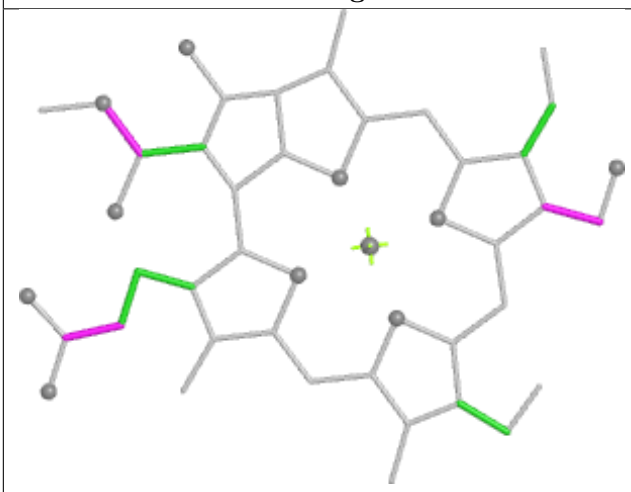
Ligand CHL 1 312



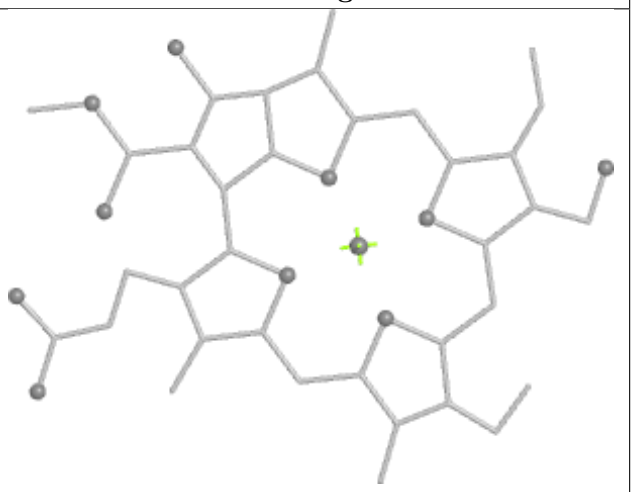
Bond lengths



Bond angles

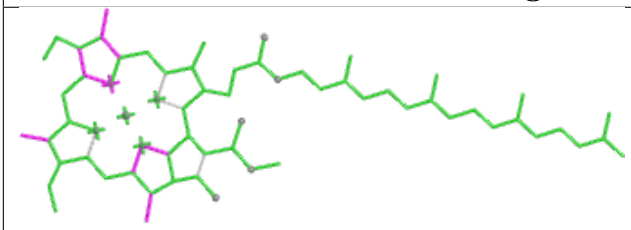


Torsions

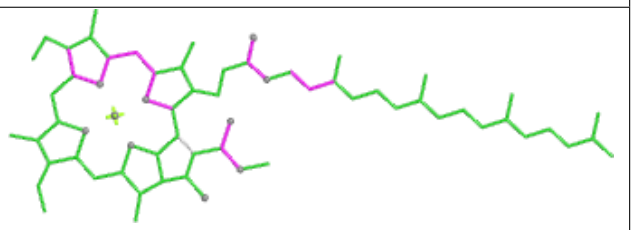


Rings

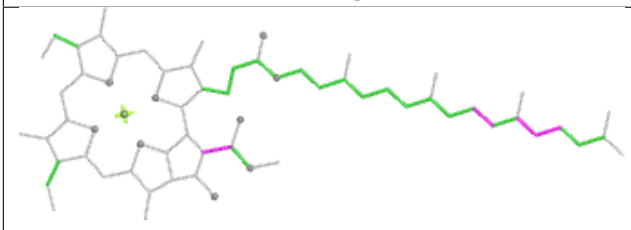
Ligand CLA B 611



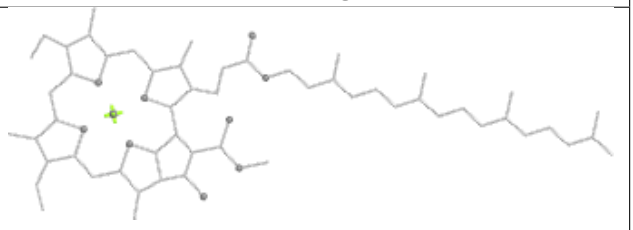
Bond lengths



Bond angles

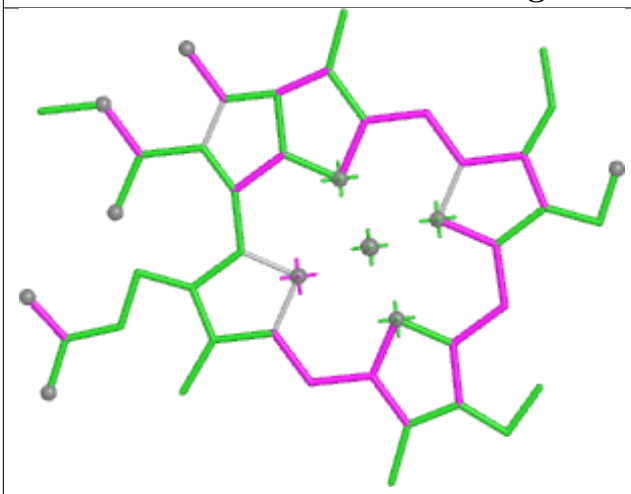


Torsions

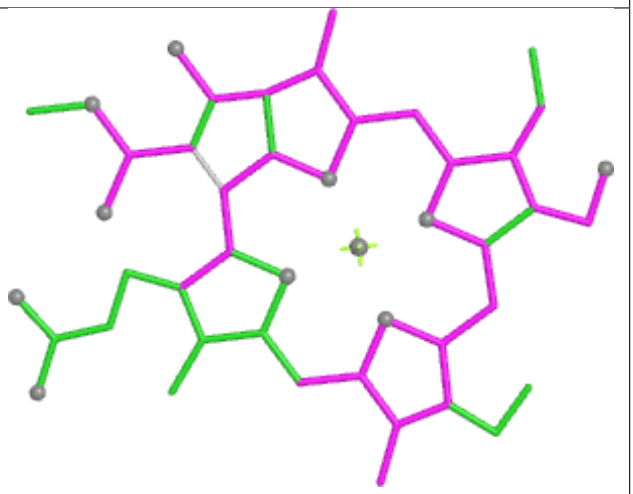


Rings

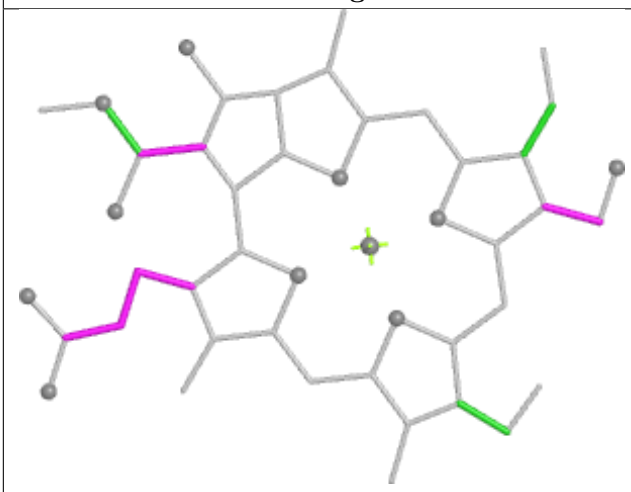
Ligand CHL 4 305



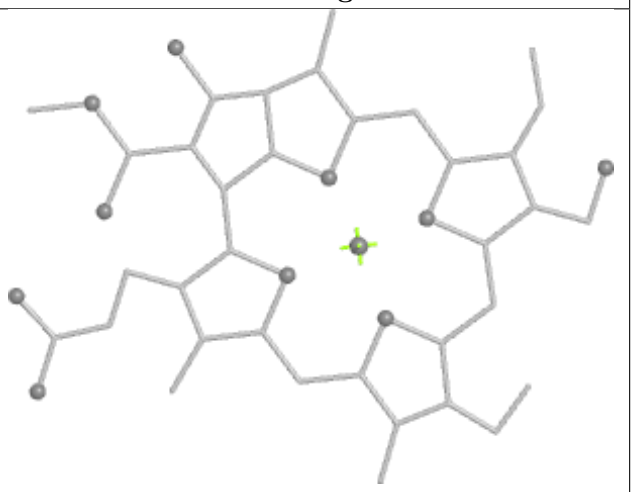
Bond lengths



Bond angles

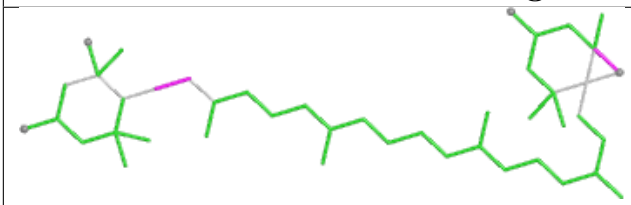


Torsions



Rings

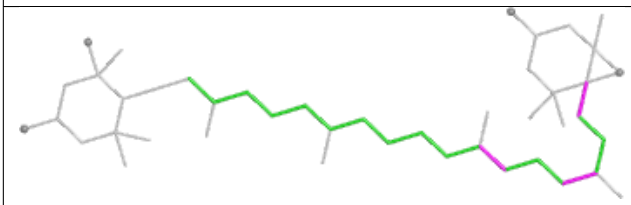
Ligand NEX 1 303



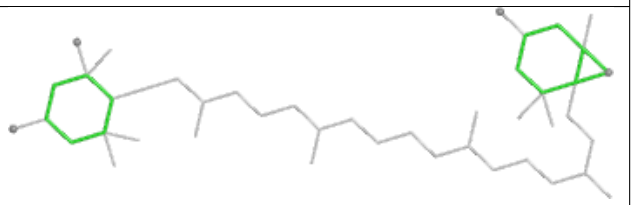
Bond lengths



Bond angles

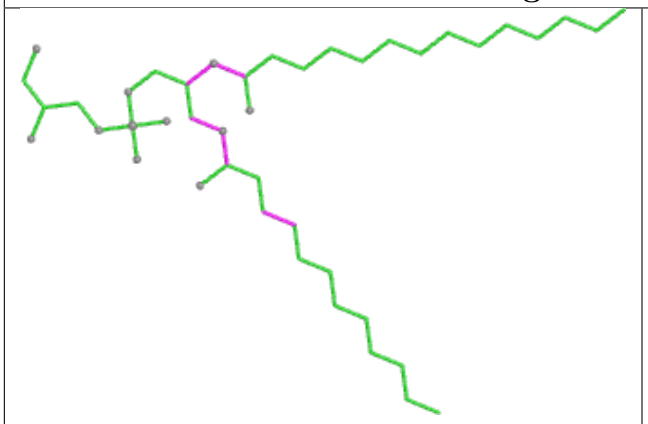


Torsions

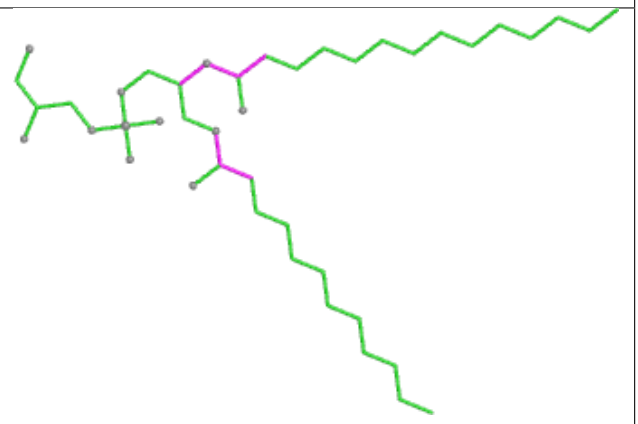


Rings

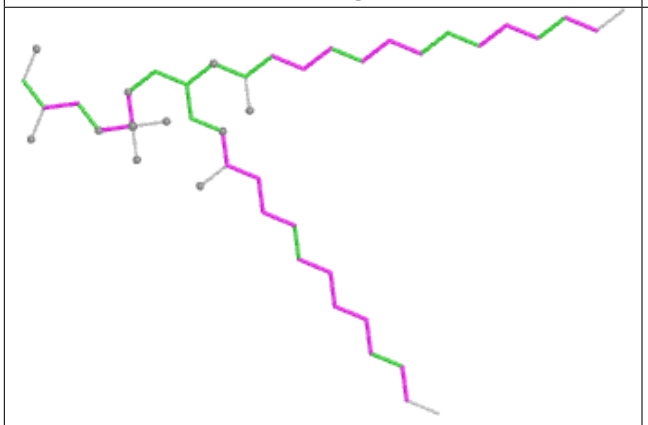
Ligand LHG Y 318



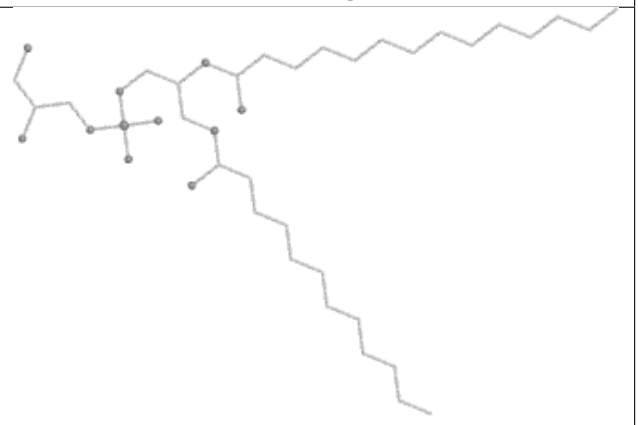
Bond lengths



Bond angles

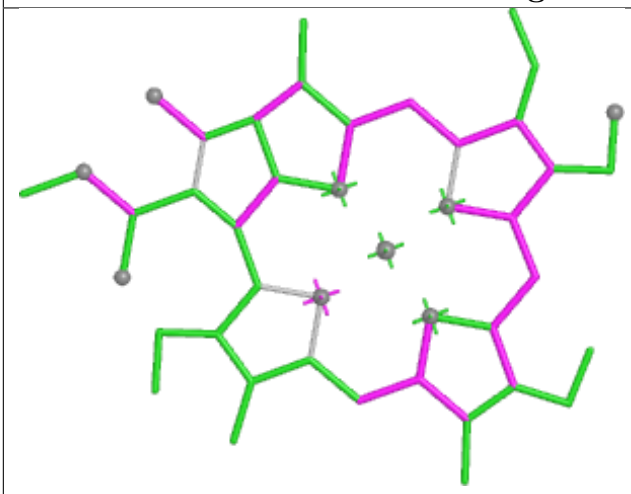


Torsions

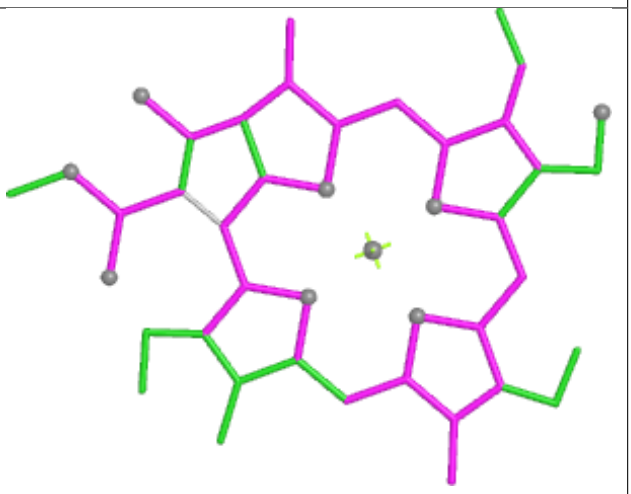


Rings

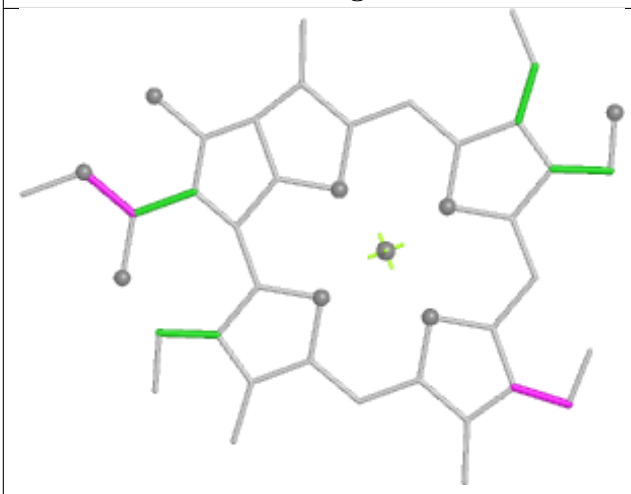
Ligand CHL 3 308



Bond lengths



Bond angles

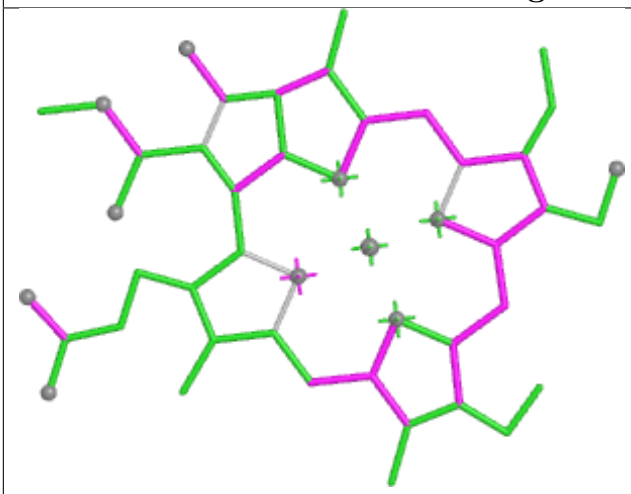


Torsions

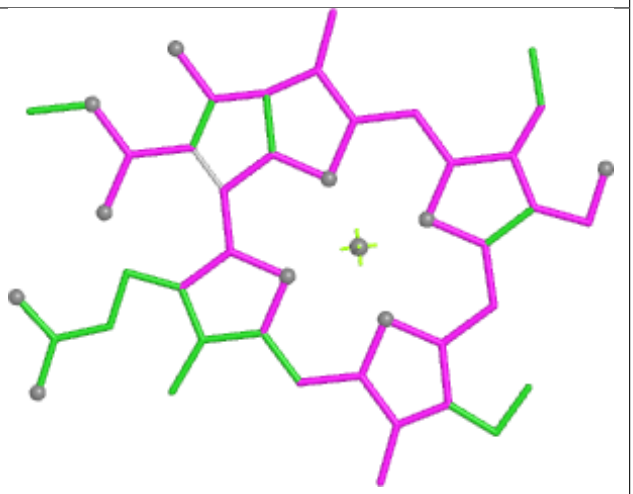


Rings

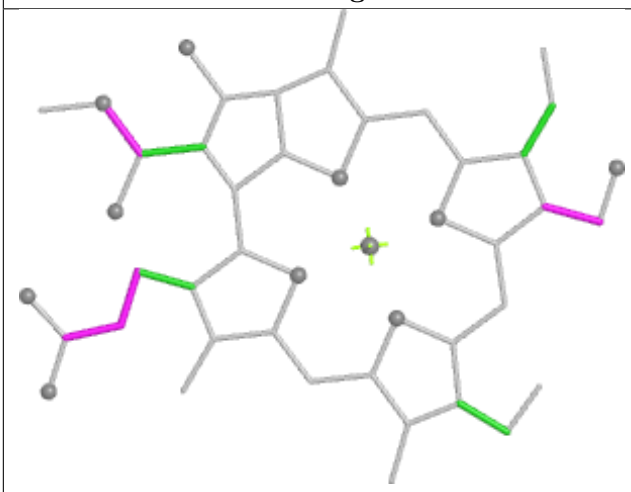
Ligand CHL 7 310



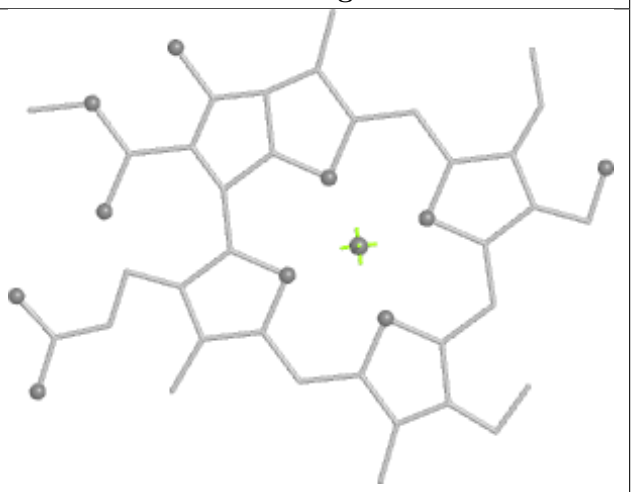
Bond lengths



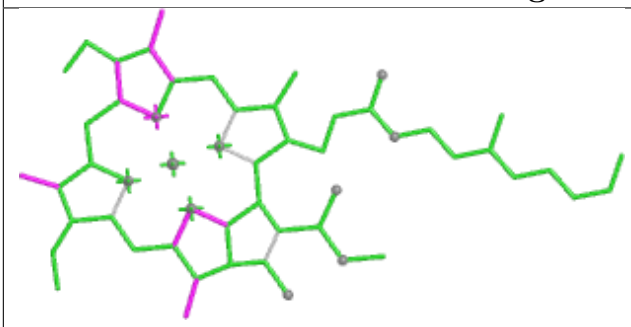
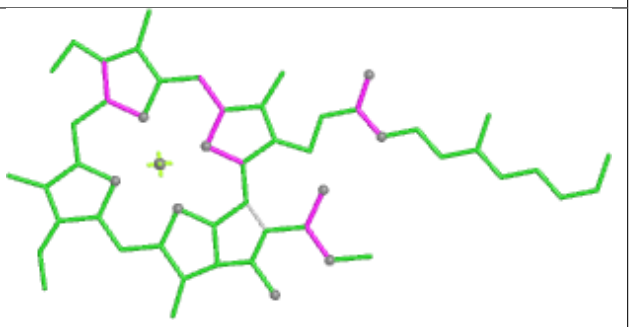
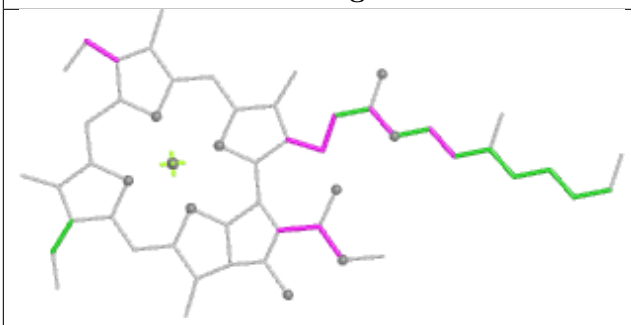
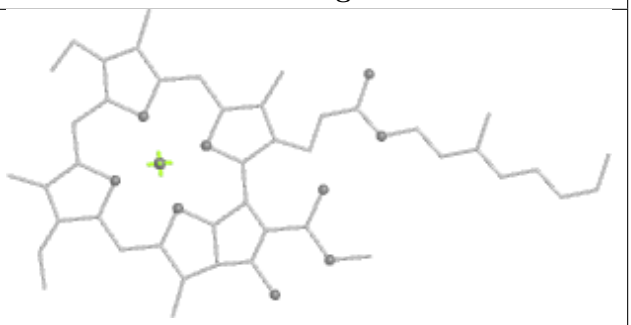
Bond angles

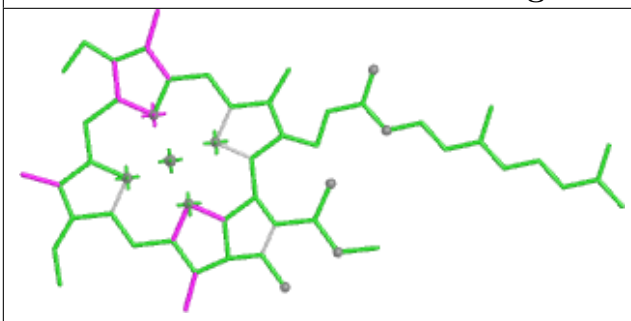
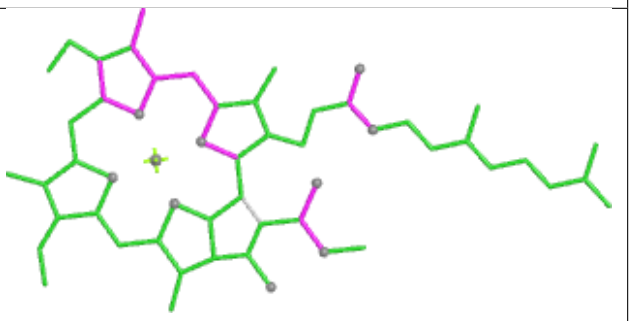
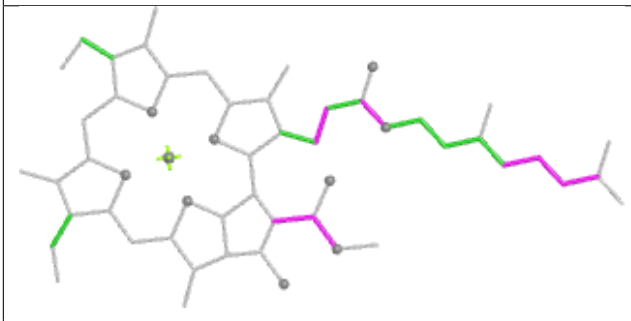
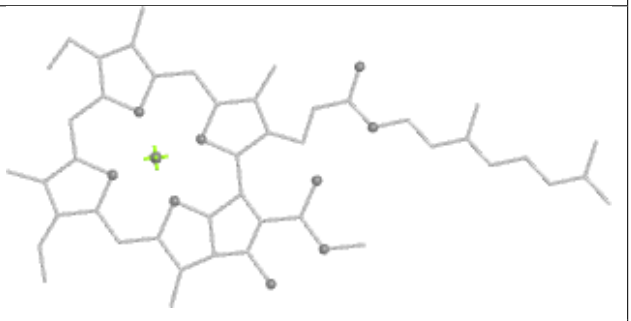


Torsions

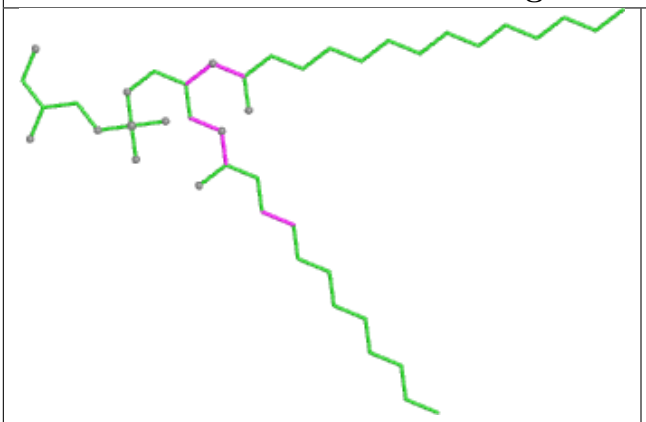


Rings

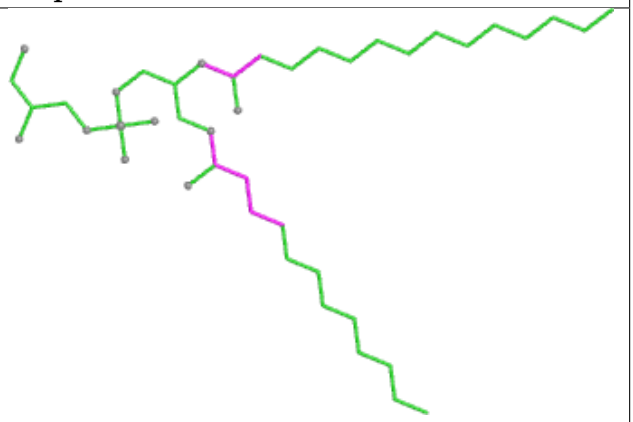
Ligand CLA 8 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

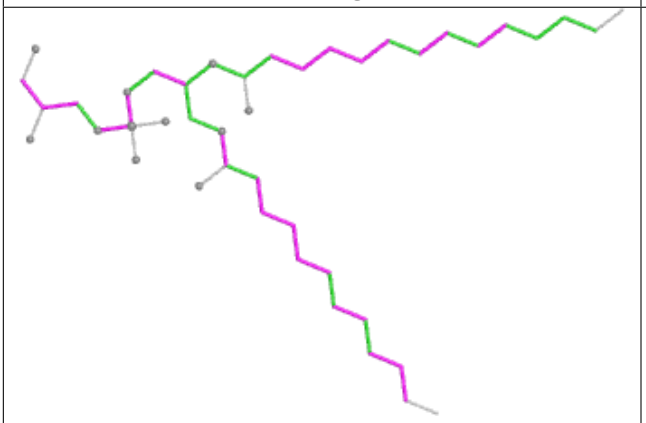
Ligand LHG p 319



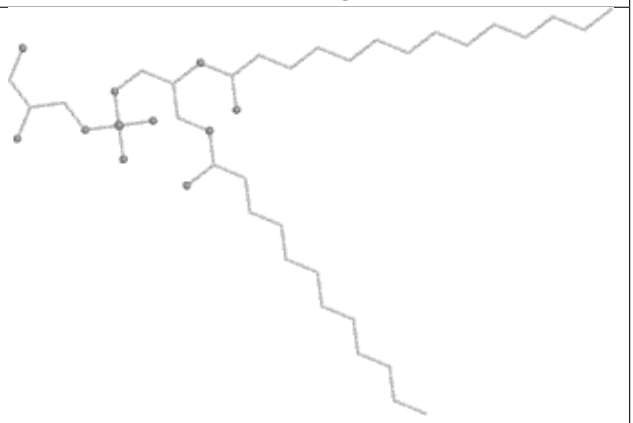
Bond lengths



Bond angles

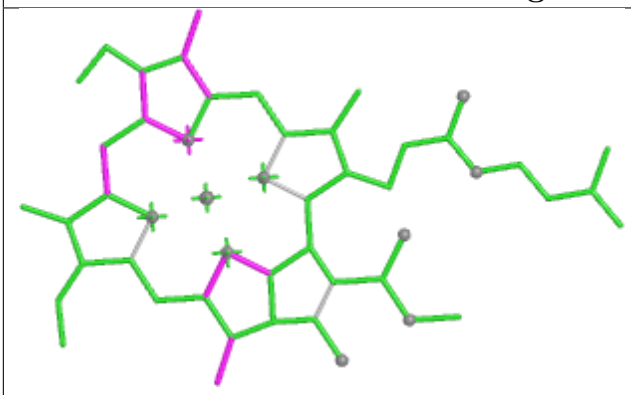


Torsions

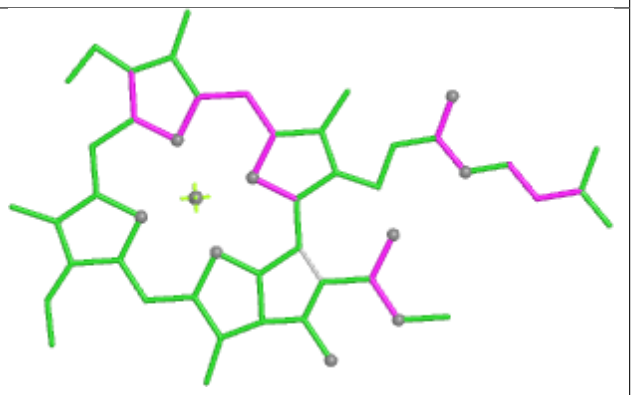


Rings

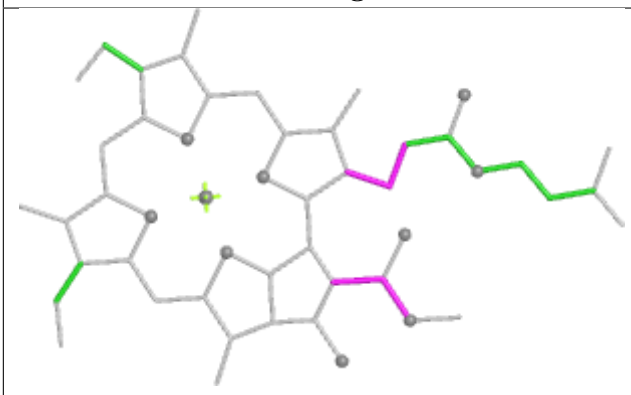
Ligand CLA u 308



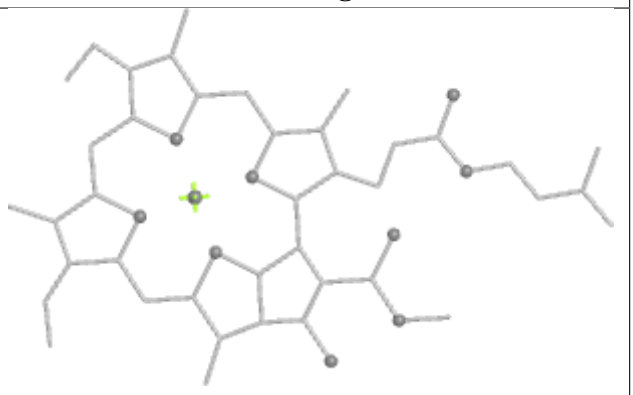
Bond lengths



Bond angles

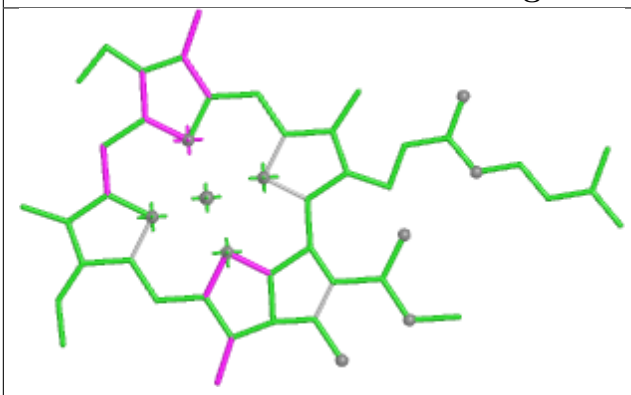


Torsions

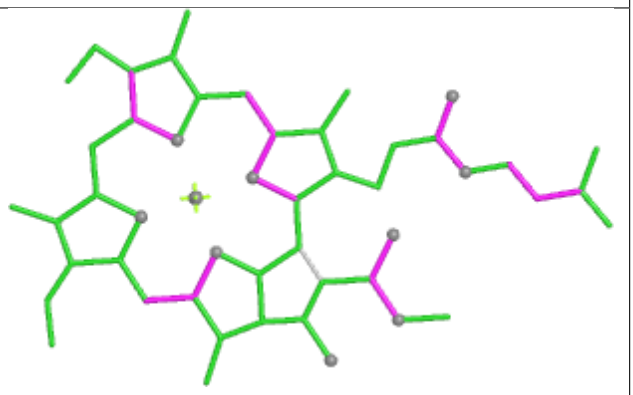


Rings

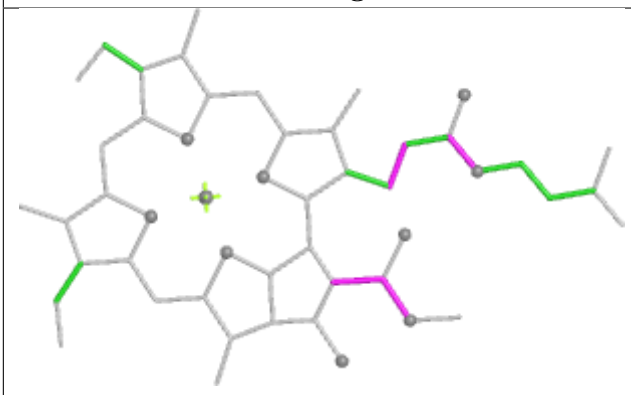
Ligand CLA N 307



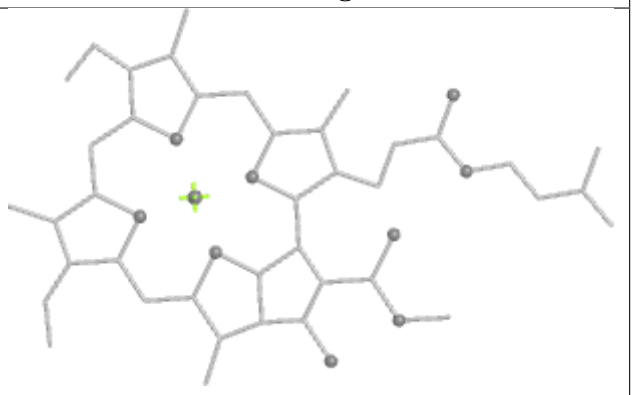
Bond lengths



Bond angles

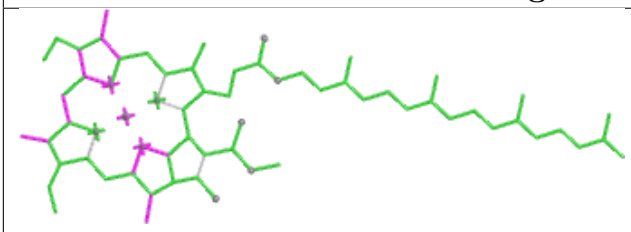


Torsions

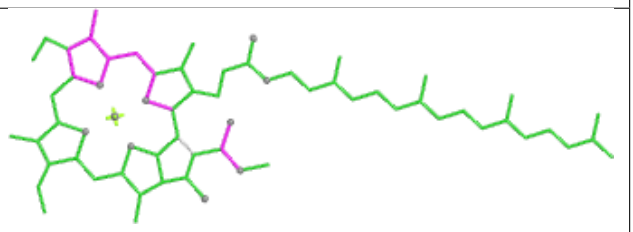


Rings

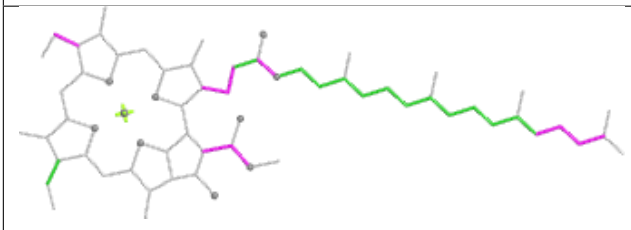
Ligand CLA a 603



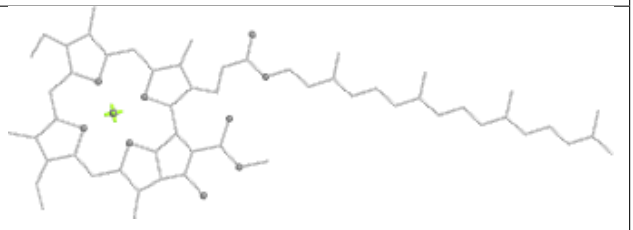
Bond lengths



Bond angles

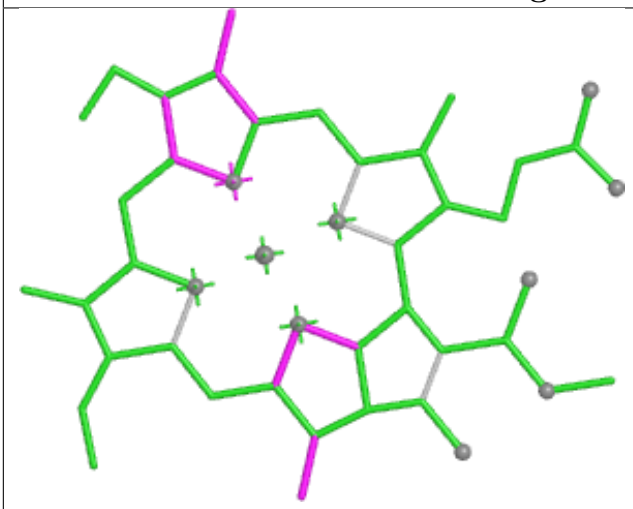


Torsions

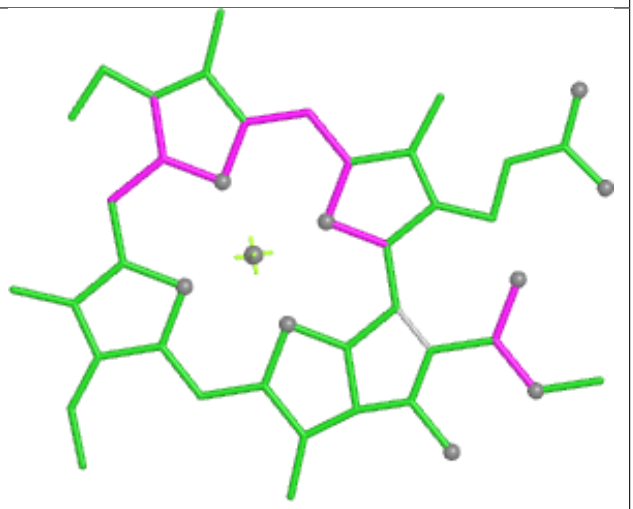


Rings

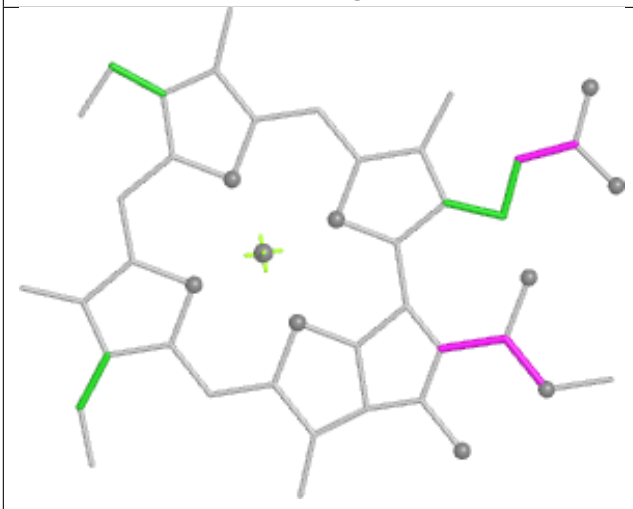
Ligand CLA s 404



Bond lengths



Bond angles

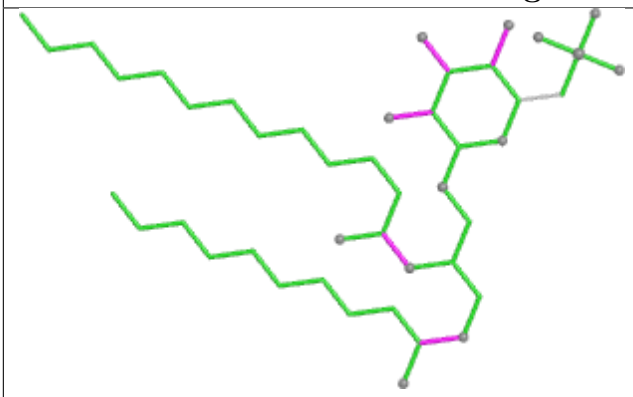


Torsions

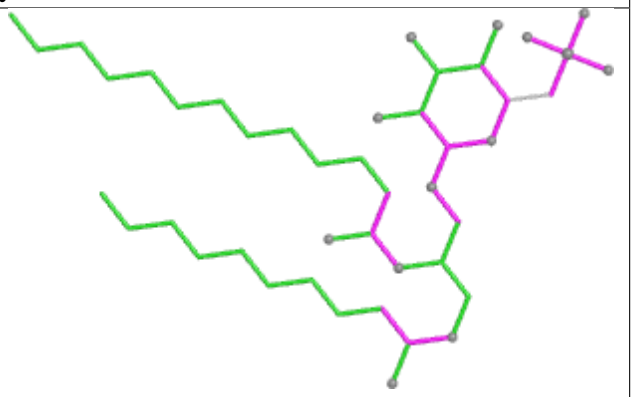


Rings

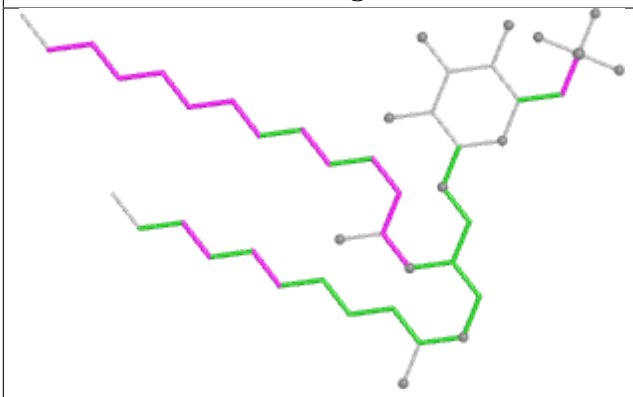
Ligand SQD A 609



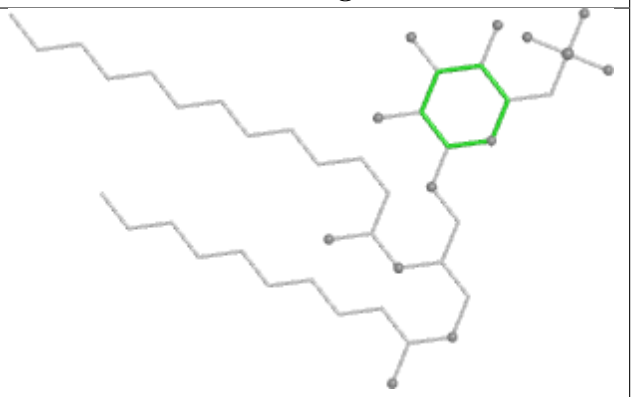
Bond lengths



Bond angles

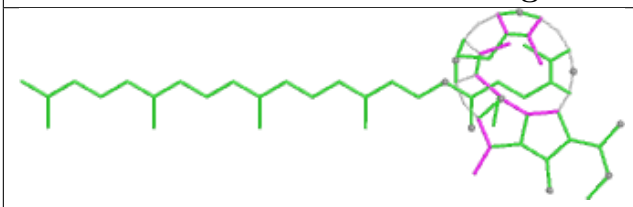


Torsions

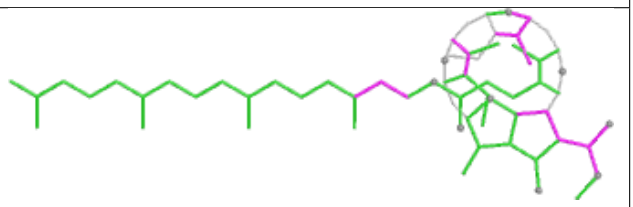


Rings

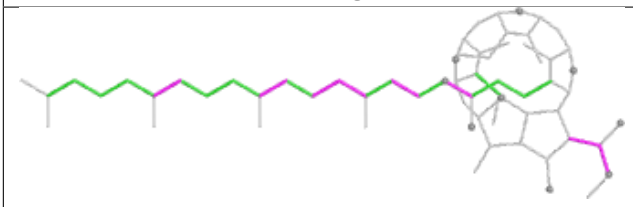
Ligand PHO D 403



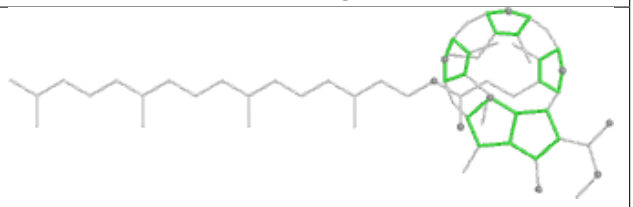
Bond lengths



Bond angles

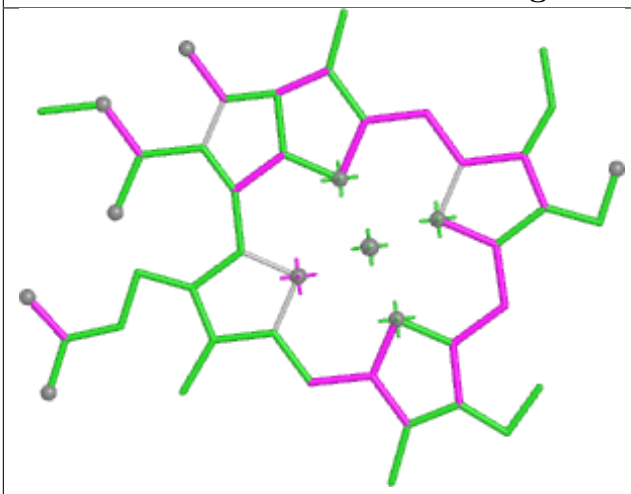


Torsions

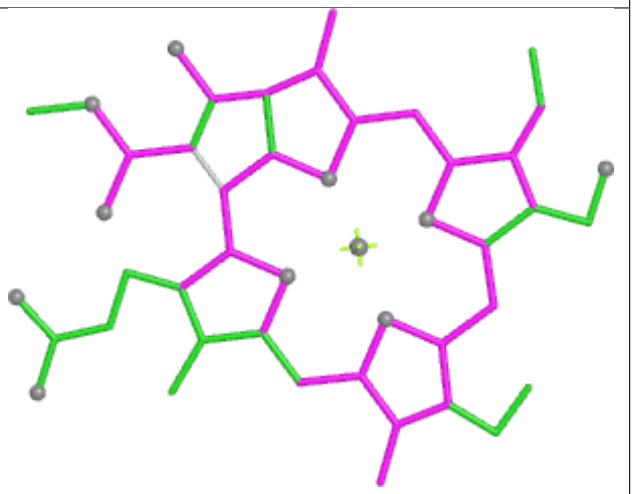


Rings

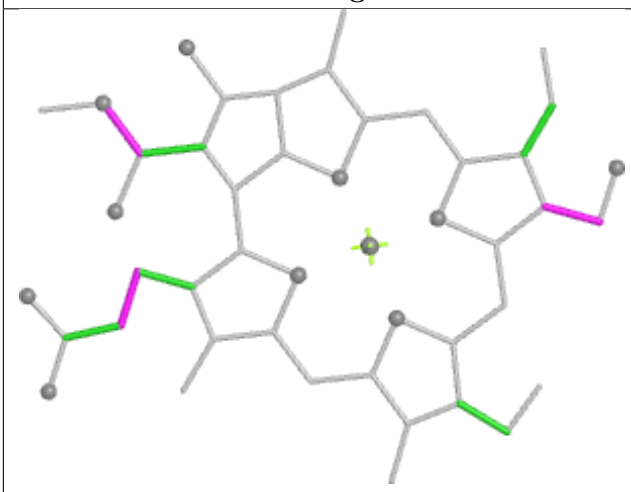
Ligand CHL r 302



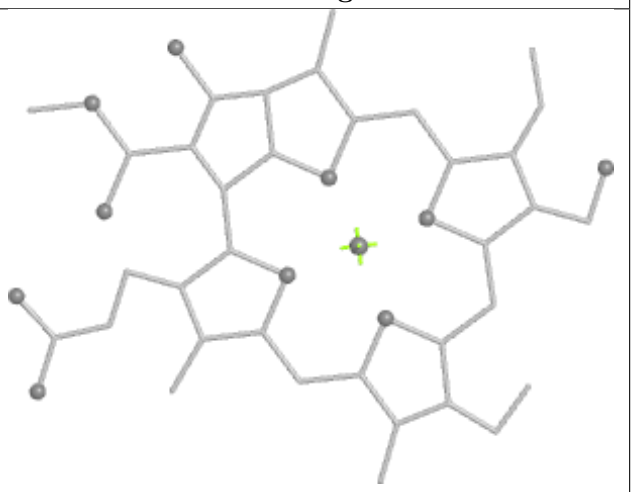
Bond lengths



Bond angles

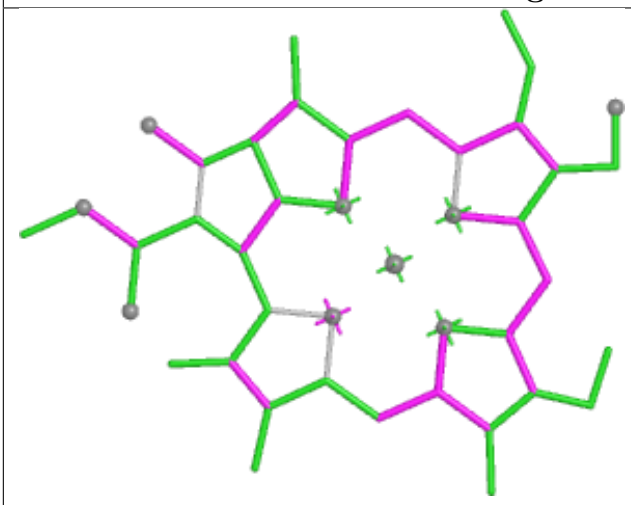


Torsions

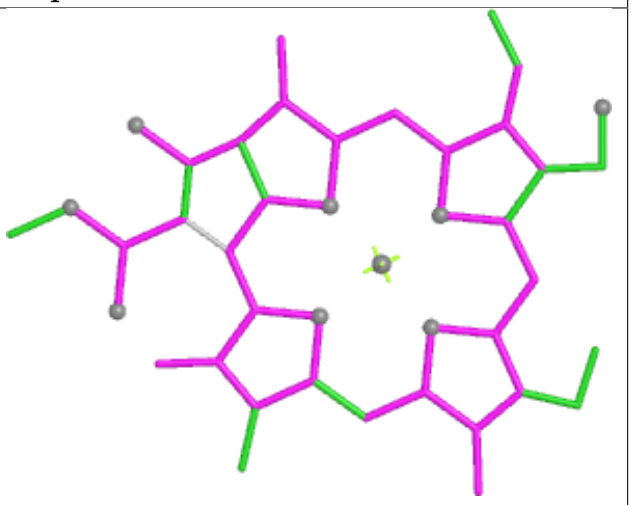


Rings

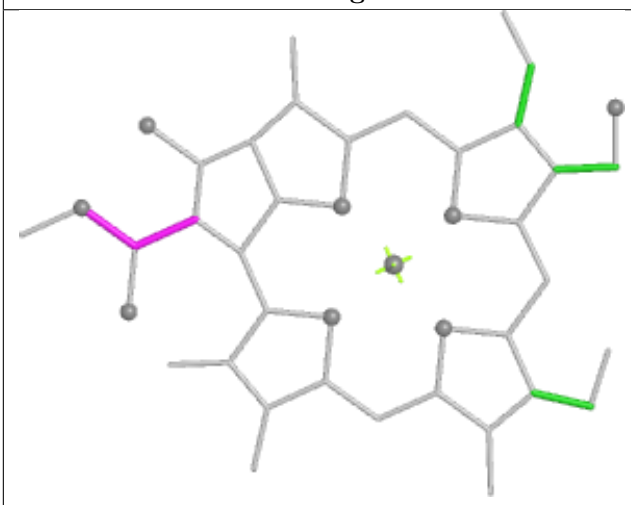
Ligand CHL p 318



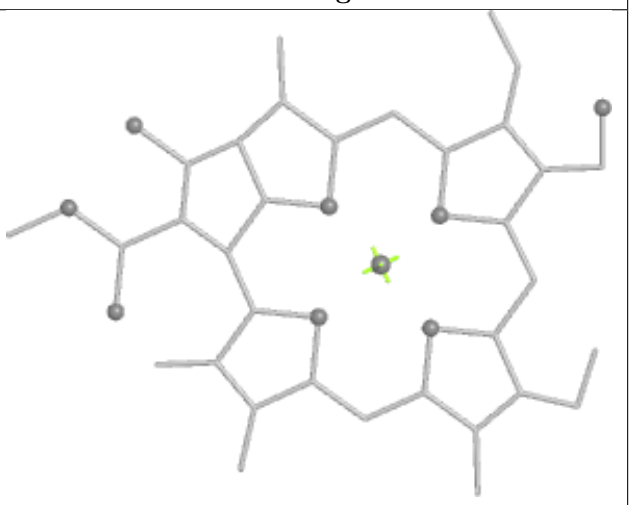
Bond lengths



Bond angles

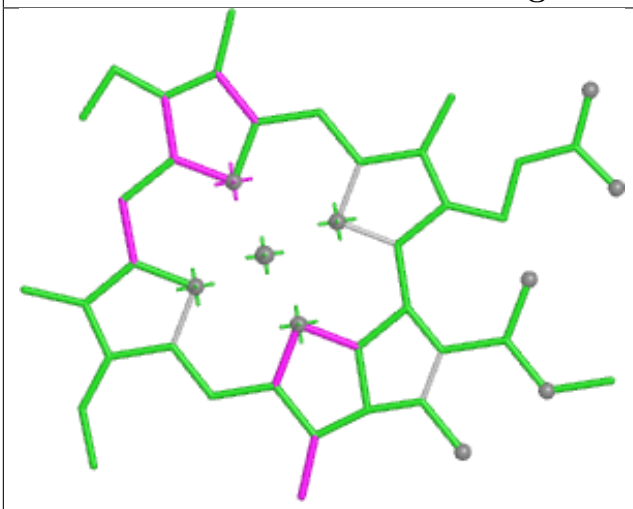


Torsions

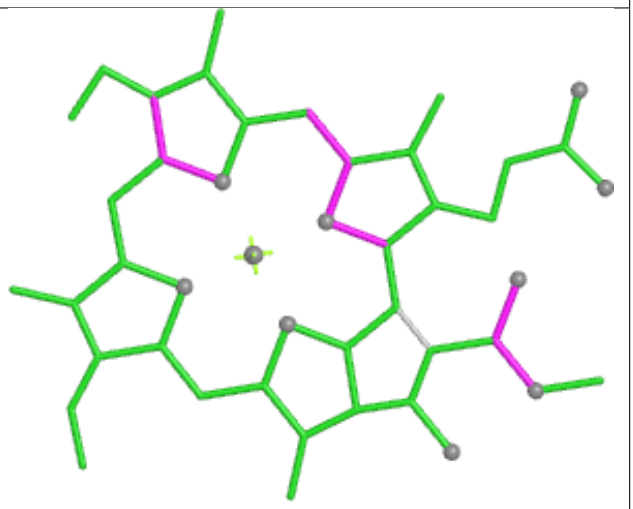


Rings

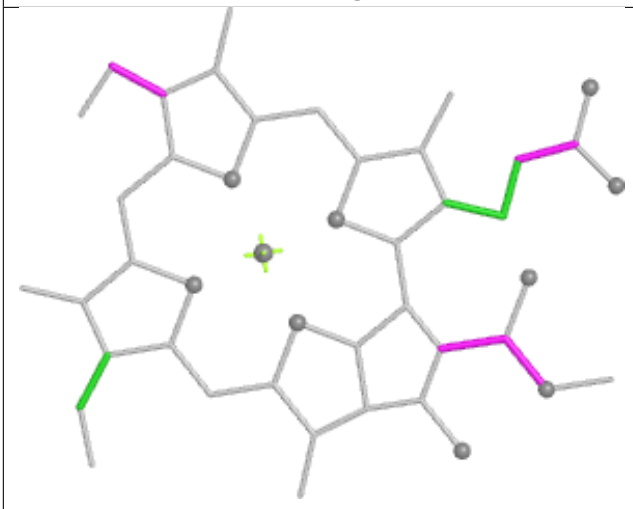
Ligand CLA 1 315



Bond lengths



Bond angles

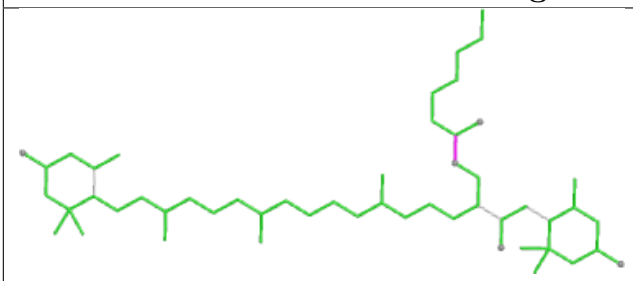


Torsions

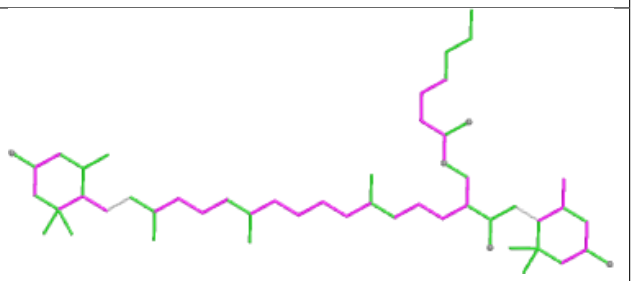


Rings

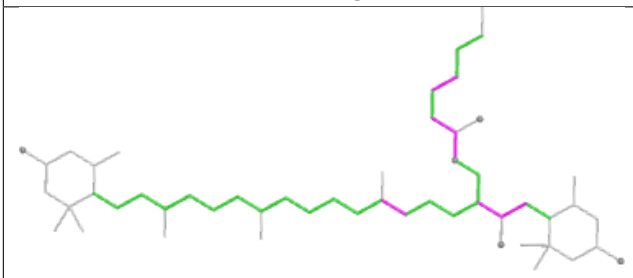
Ligand 0UR 8 301



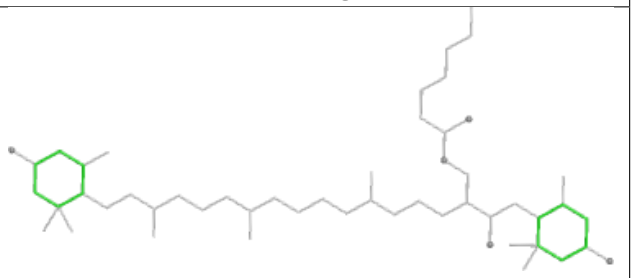
Bond lengths



Bond angles

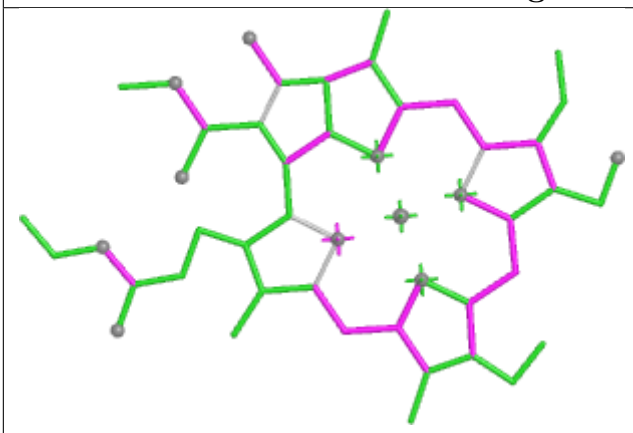


Torsions

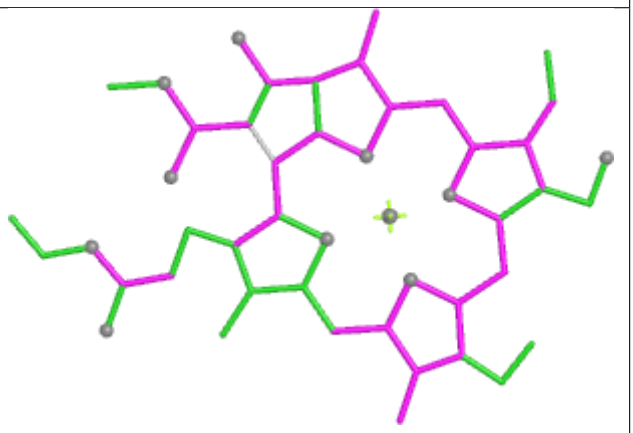


Rings

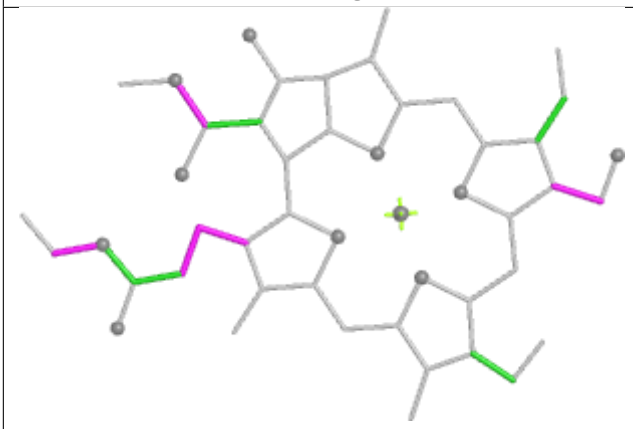
Ligand CHL 3 304



Bond lengths



Bond angles

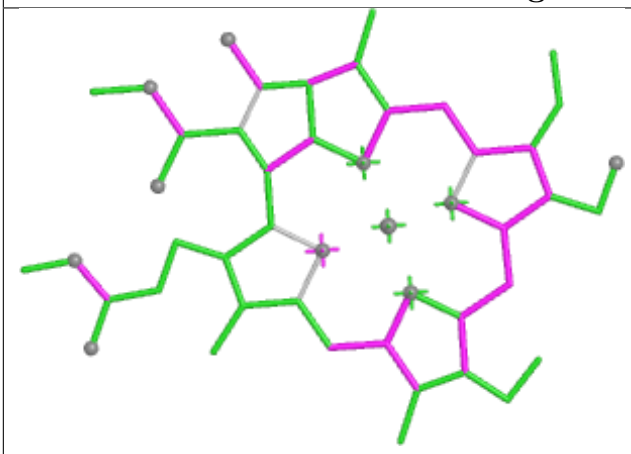


Torsions

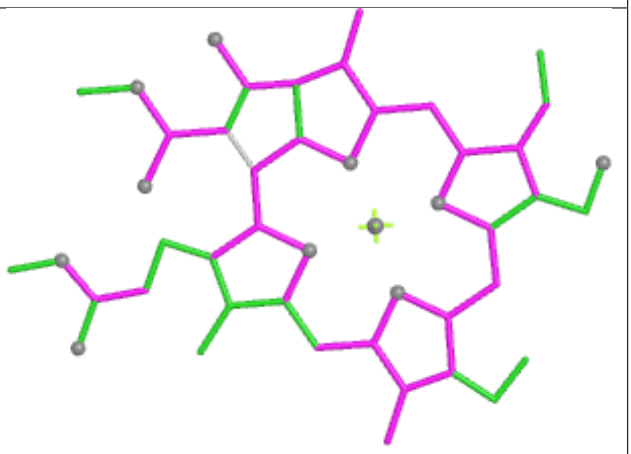


Rings

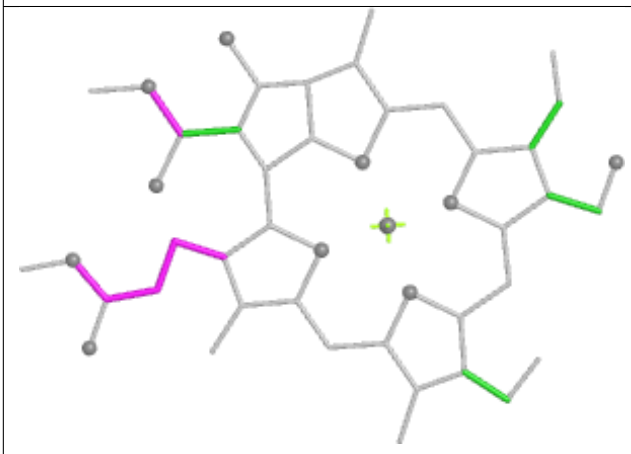
Ligand CHL 5 311



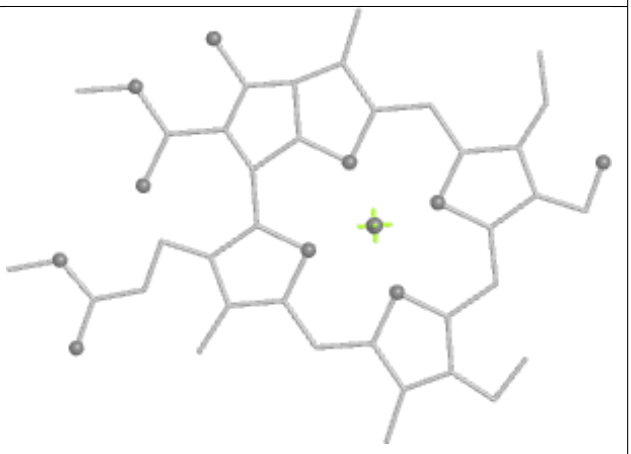
Bond lengths



Bond angles

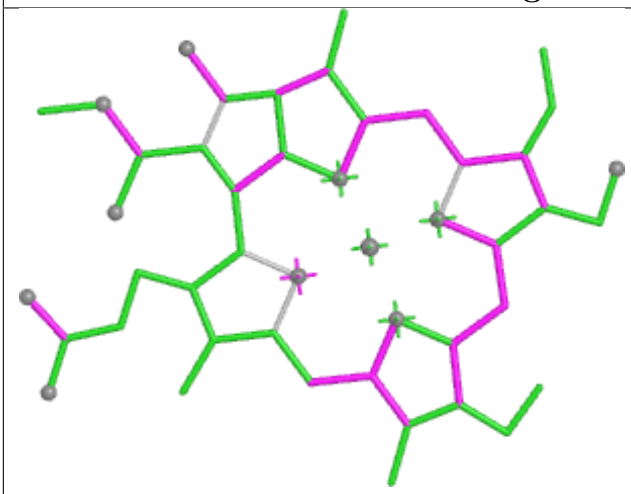


Torsions

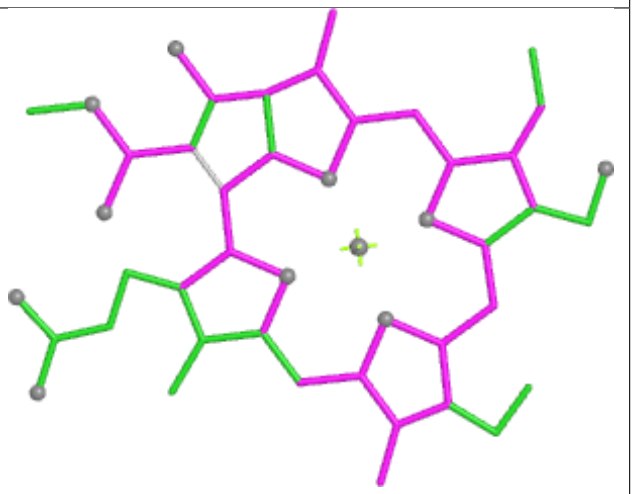


Rings

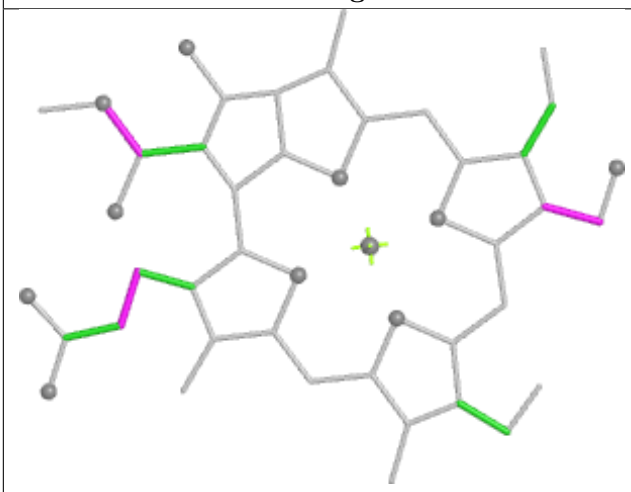
Ligand CHL R 601



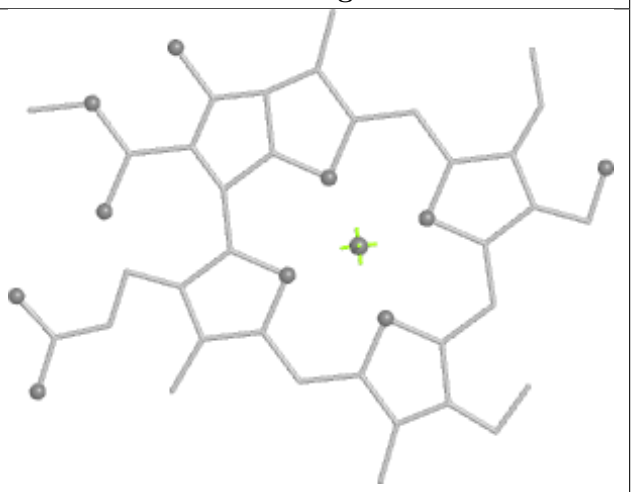
Bond lengths



Bond angles

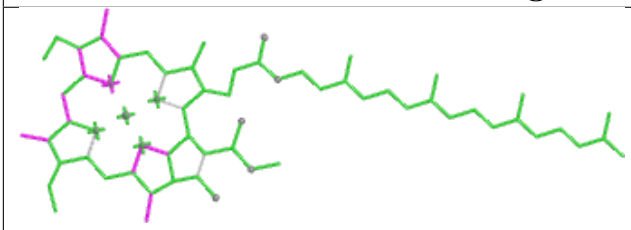


Torsions

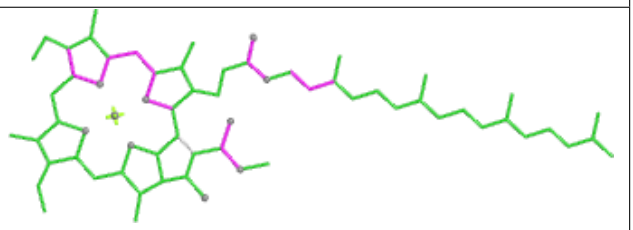


Rings

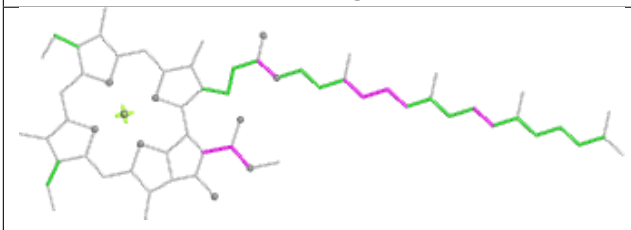
Ligand CLA b 613



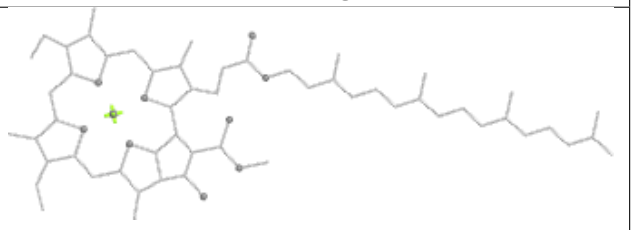
Bond lengths



Bond angles

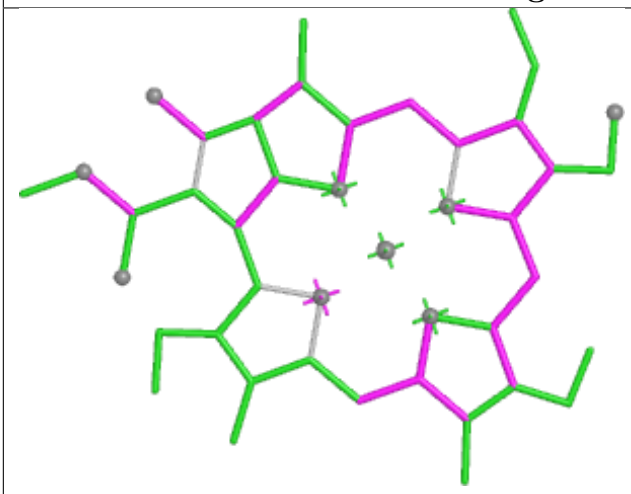


Torsions

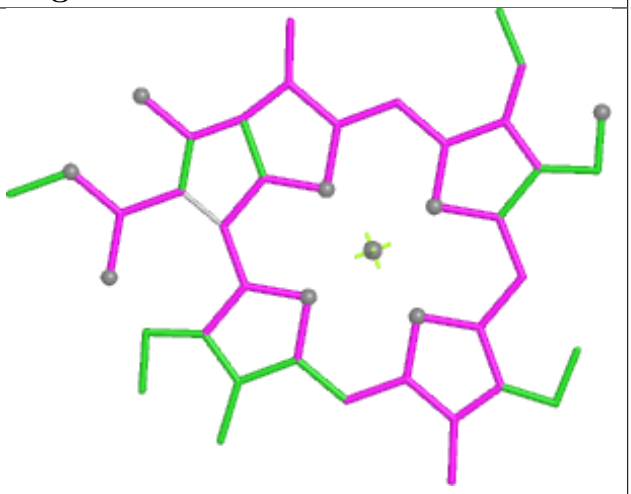


Rings

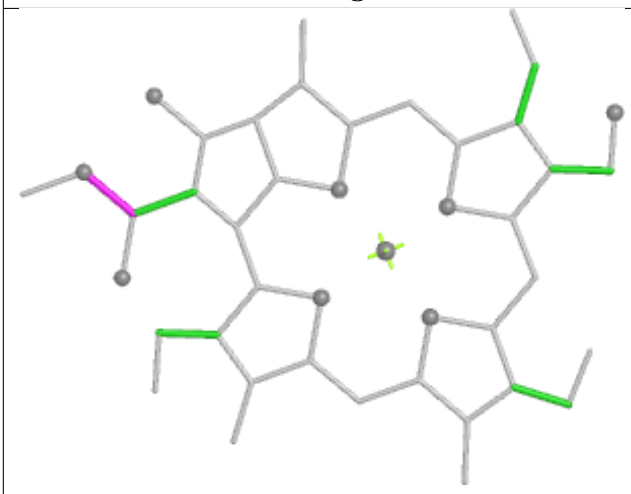
Ligand CHL g 309



Bond lengths



Bond angles

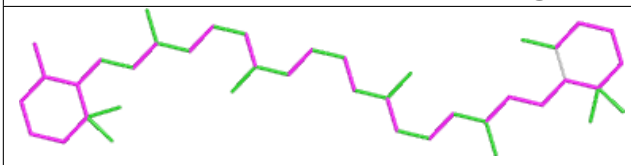


Torsions

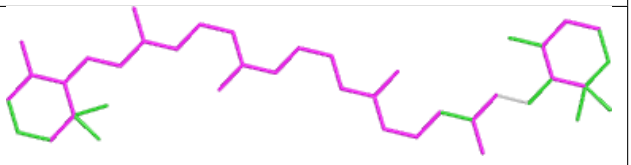


Rings

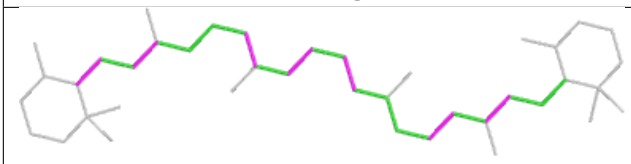
Ligand 8CT x 601



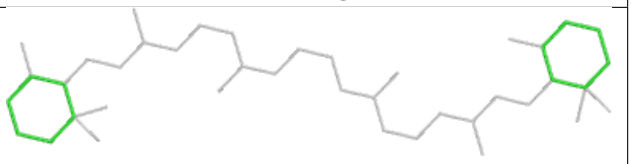
Bond lengths



Bond angles

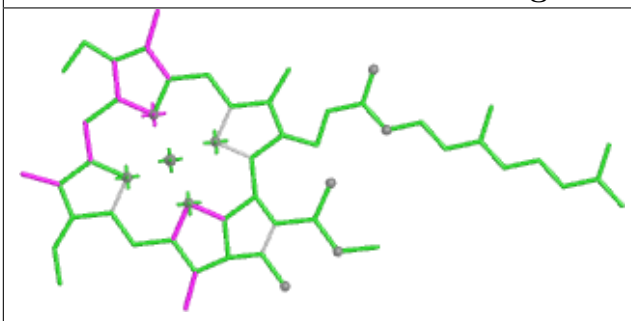


Torsions

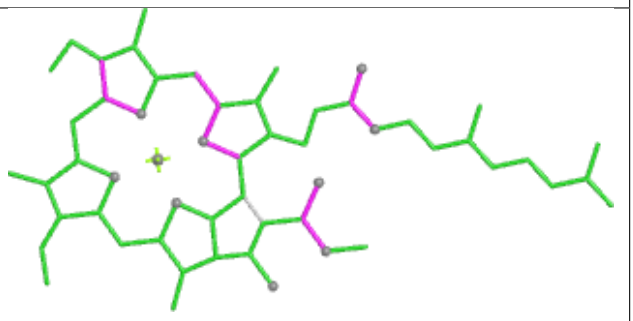


Rings

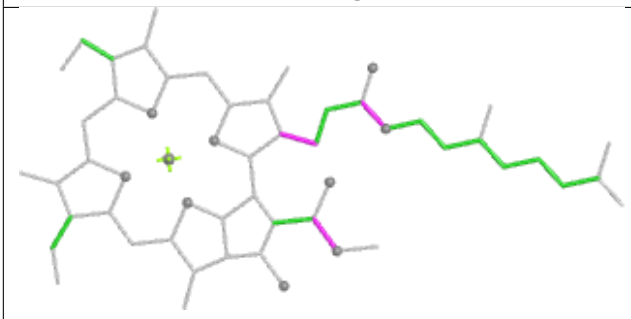
Ligand CLA r 310



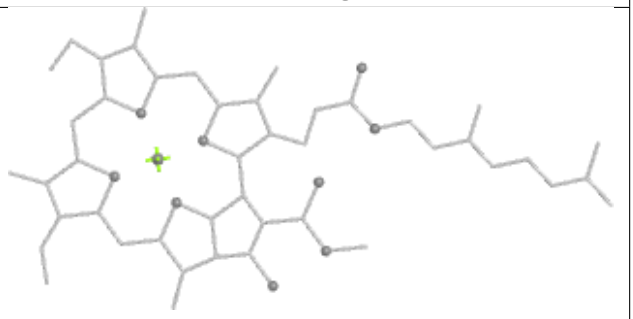
Bond lengths



Bond angles

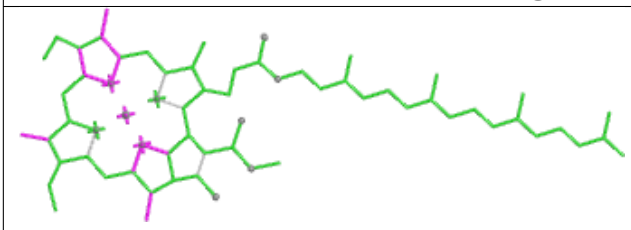


Torsions

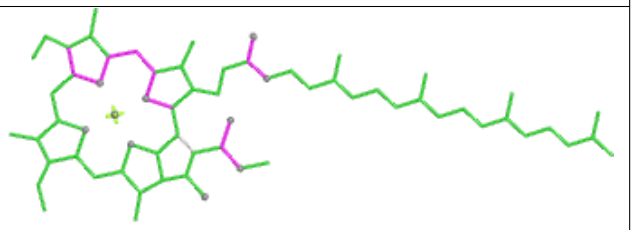


Rings

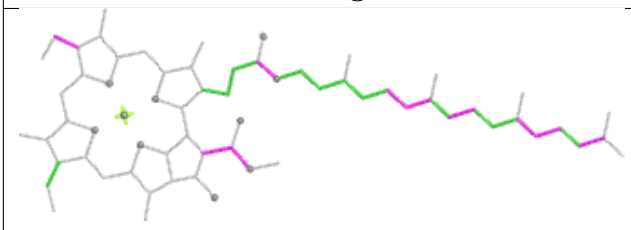
Ligand CLA c 602



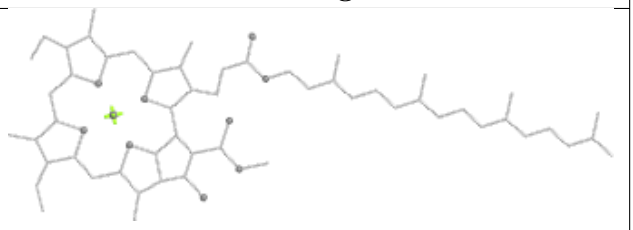
Bond lengths



Bond angles

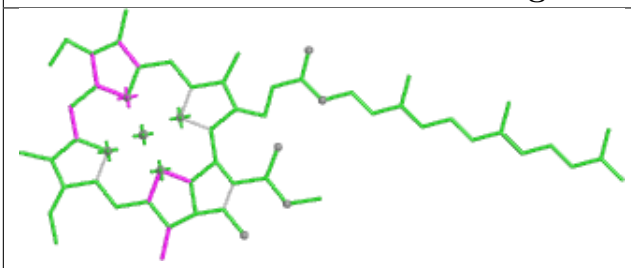


Torsions

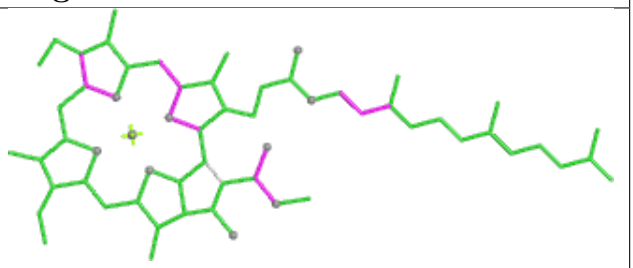


Rings

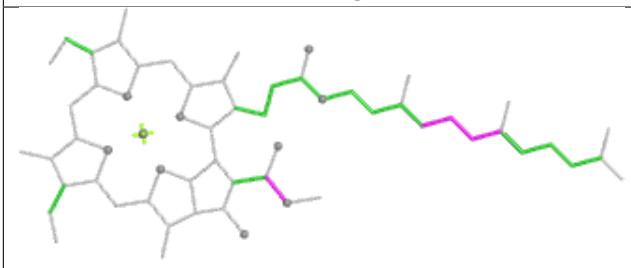
Ligand CLA g 315



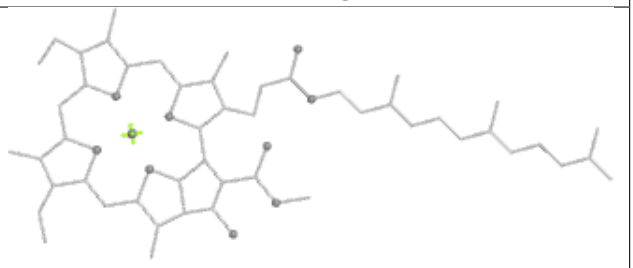
Bond lengths



Bond angles

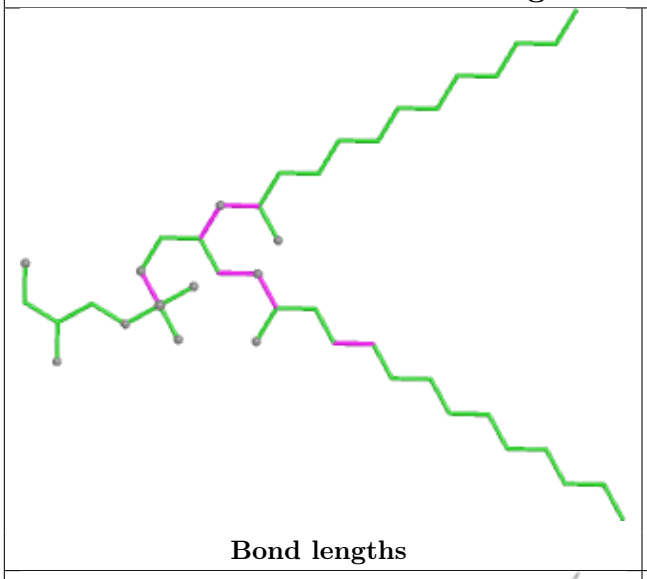


Torsions

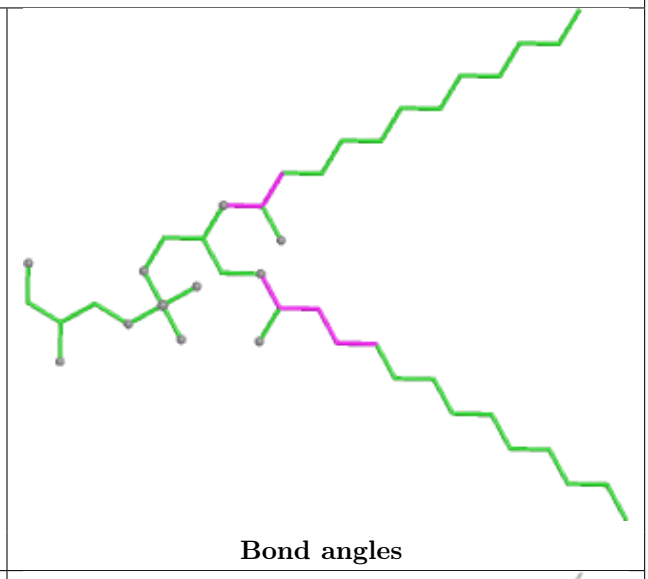


Rings

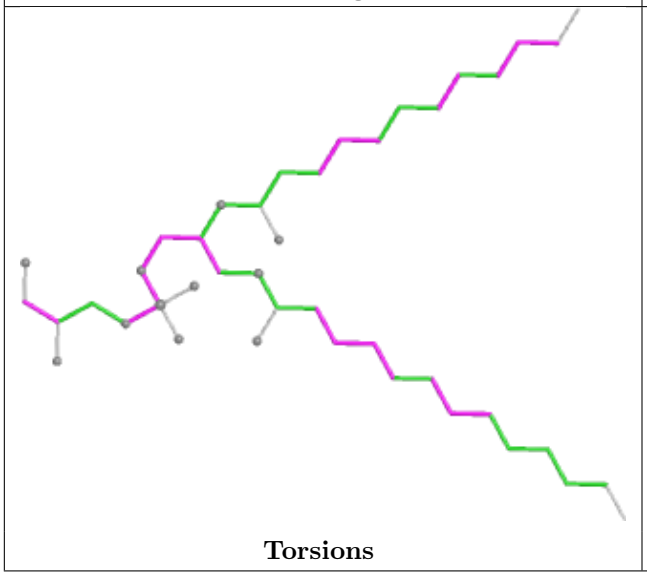
Ligand LHG 4 318



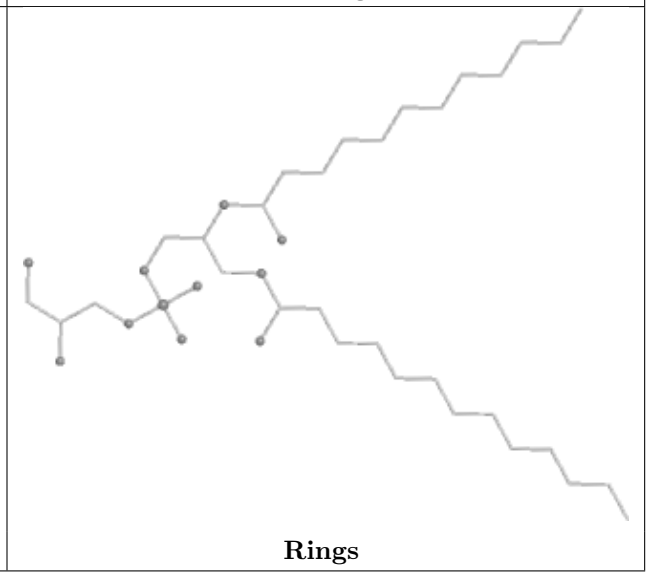
Bond lengths



Bond angles

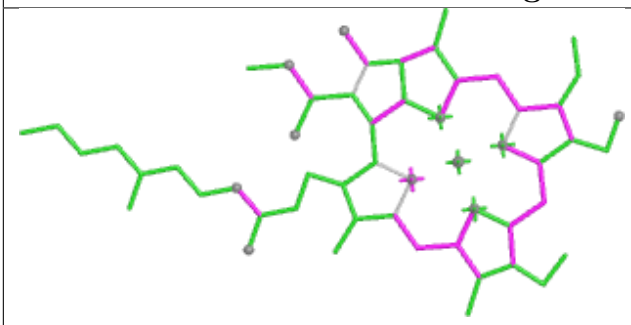


Torsions

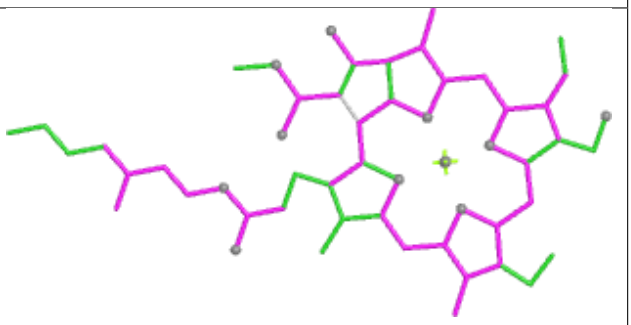


Rings

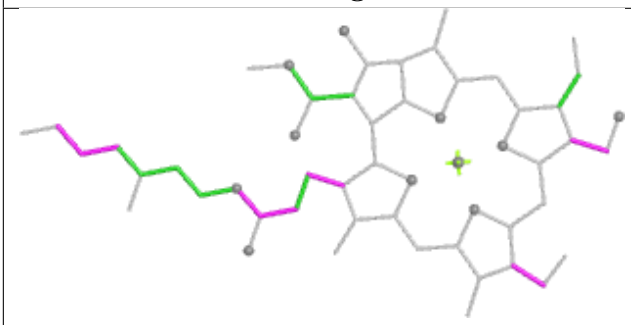
Ligand CHL Y 310



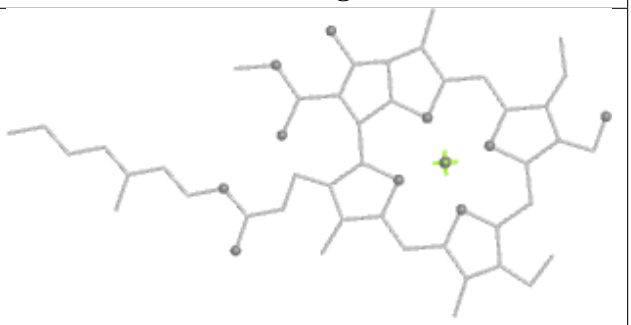
Bond lengths



Bond angles

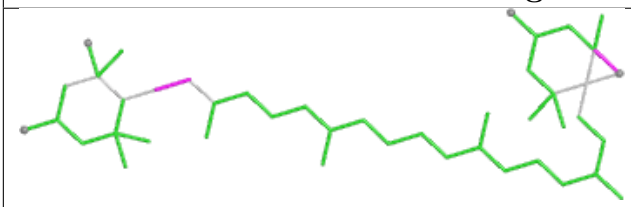


Torsions



Rings

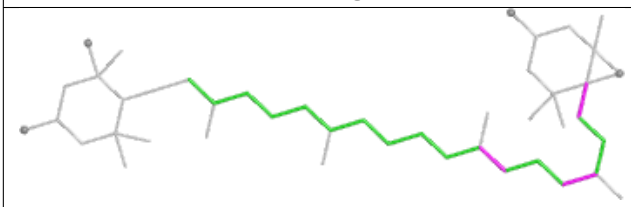
Ligand NEX y 304



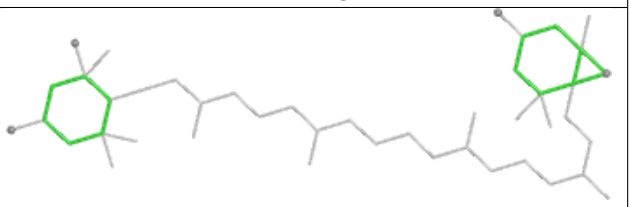
Bond lengths



Bond angles

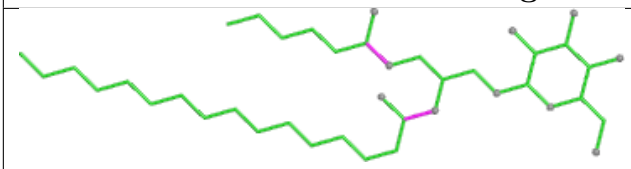


Torsions

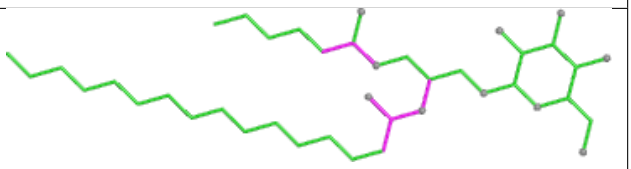


Rings

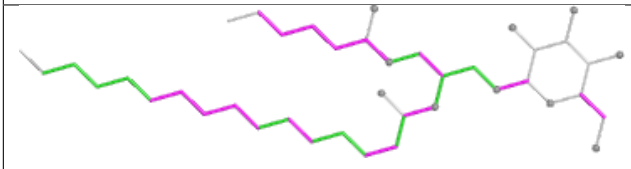
Ligand LMG B 619



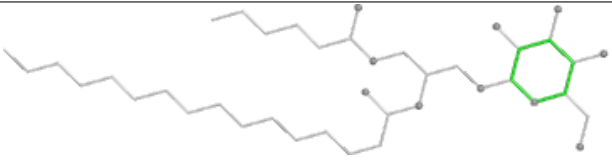
Bond lengths



Bond angles

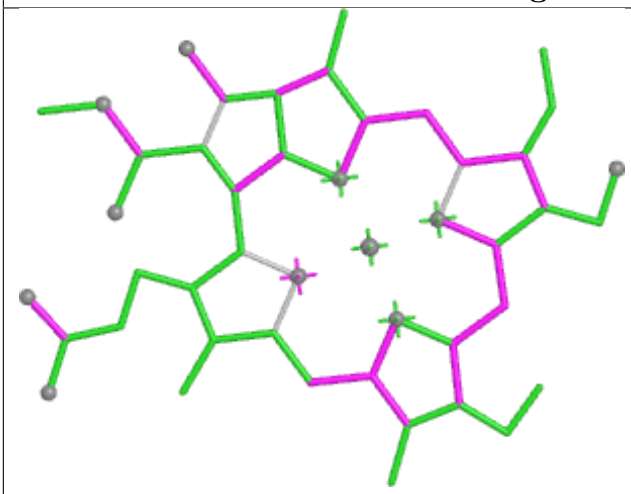


Torsions

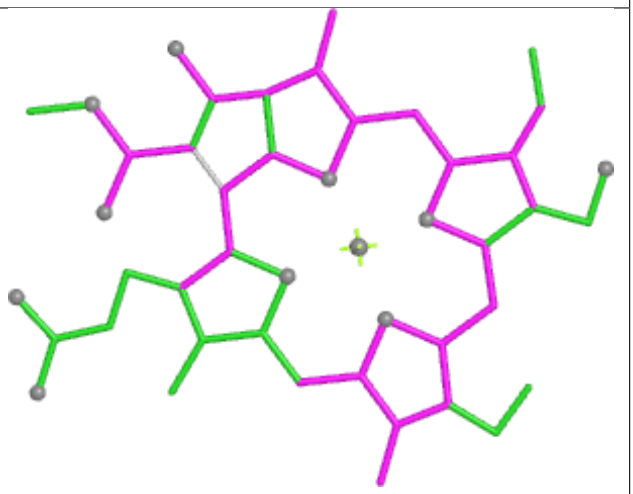


Rings

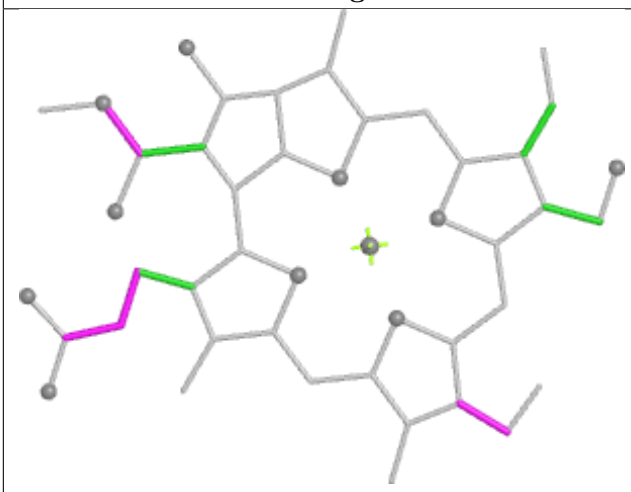
Ligand CHL s 406



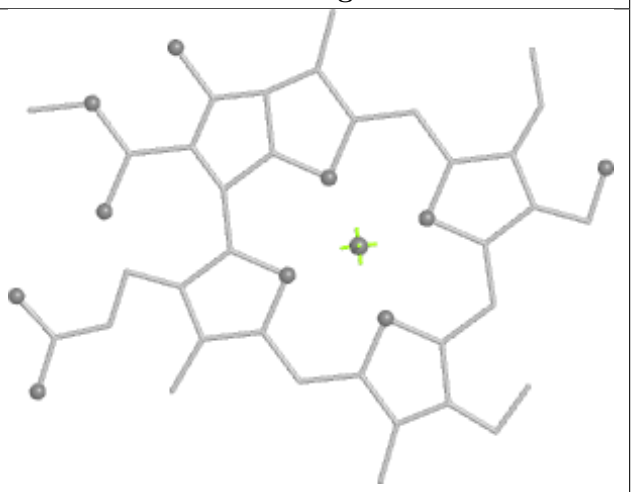
Bond lengths



Bond angles

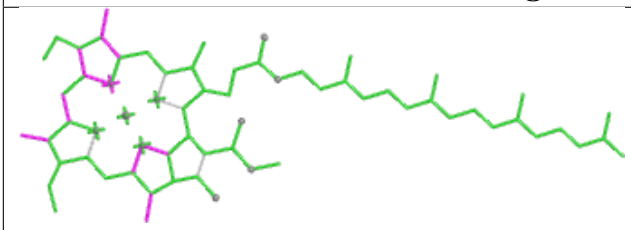


Torsions

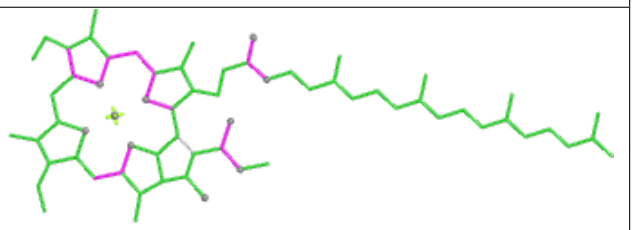


Rings

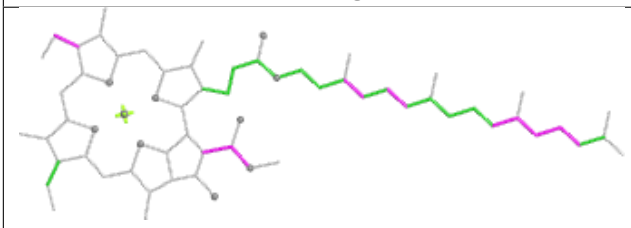
Ligand CLA B 605



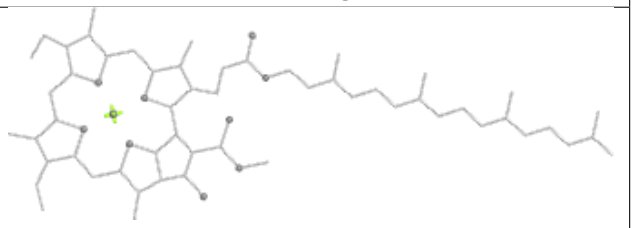
Bond lengths



Bond angles

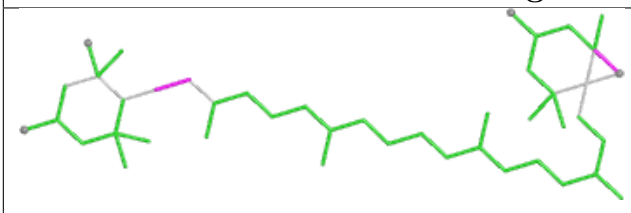


Torsions

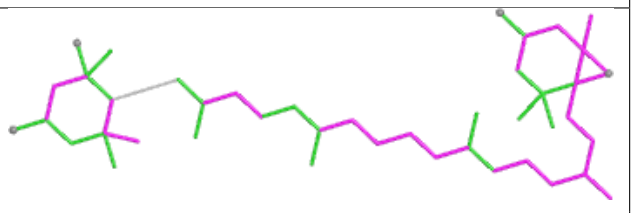


Rings

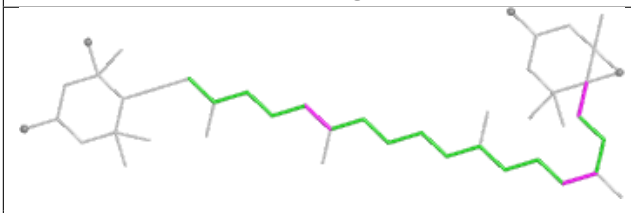
Ligand NEX 3 318



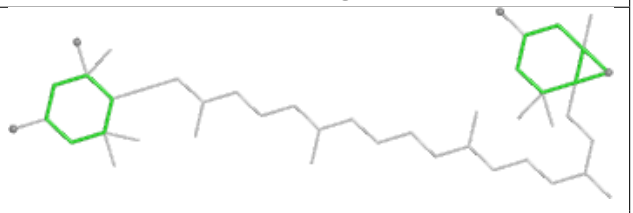
Bond lengths



Bond angles

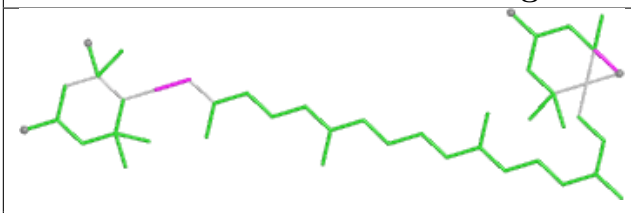


Torsions

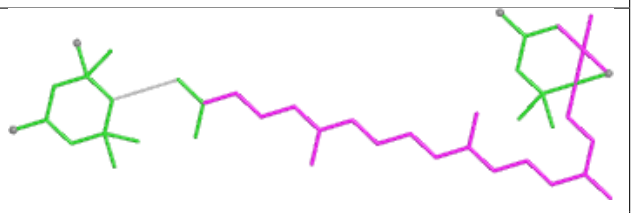


Rings

Ligand NEX G 304



Bond lengths



Bond angles

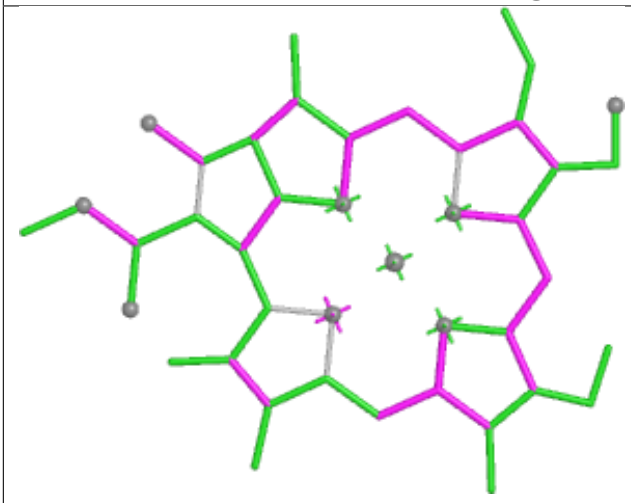


Torsions

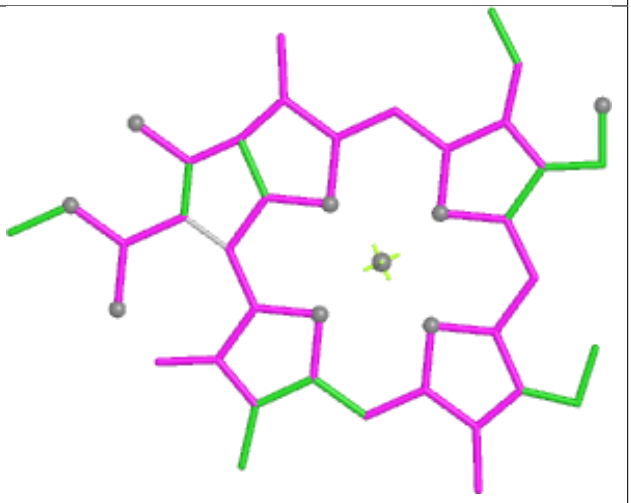


Rings

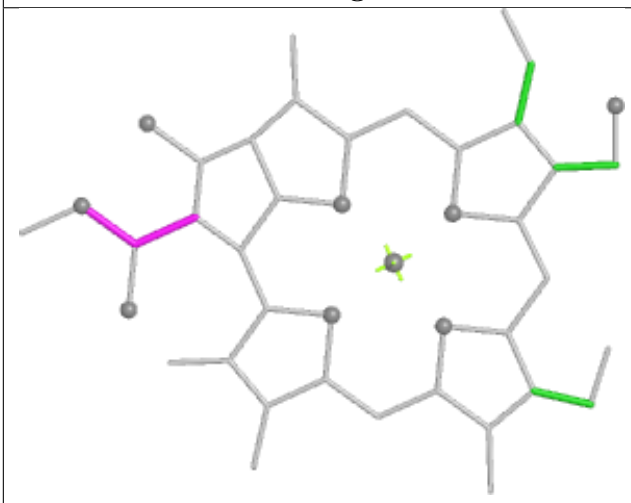
Ligand CHL 5 318



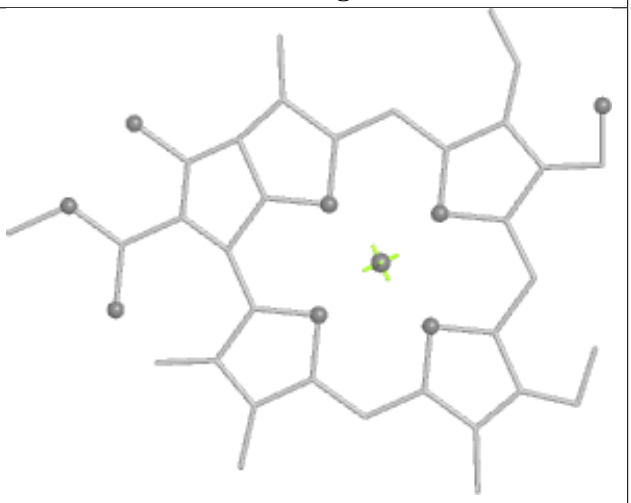
Bond lengths



Bond angles

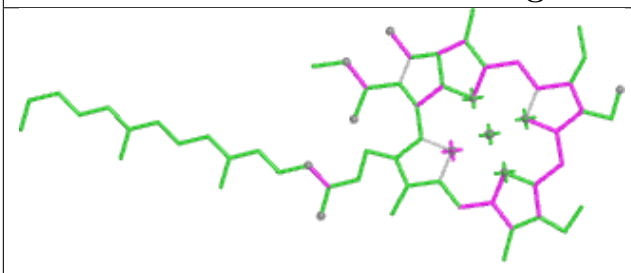


Torsions

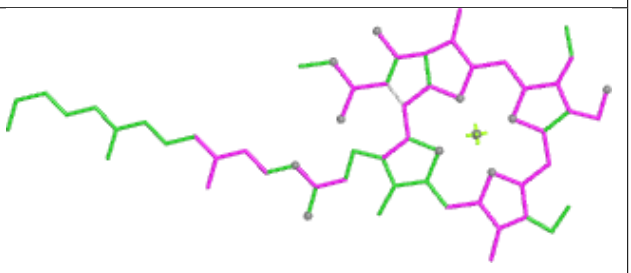


Rings

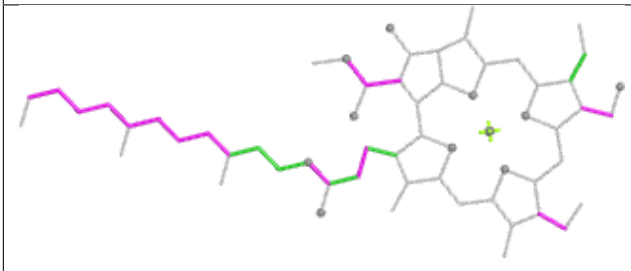
Ligand CHL n 305



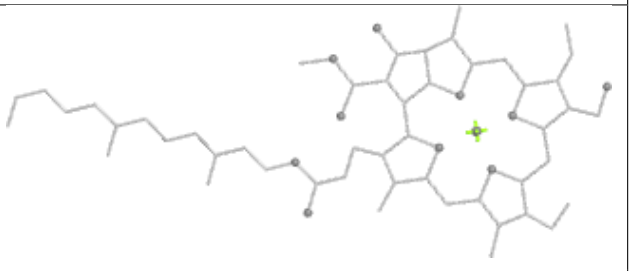
Bond lengths



Bond angles

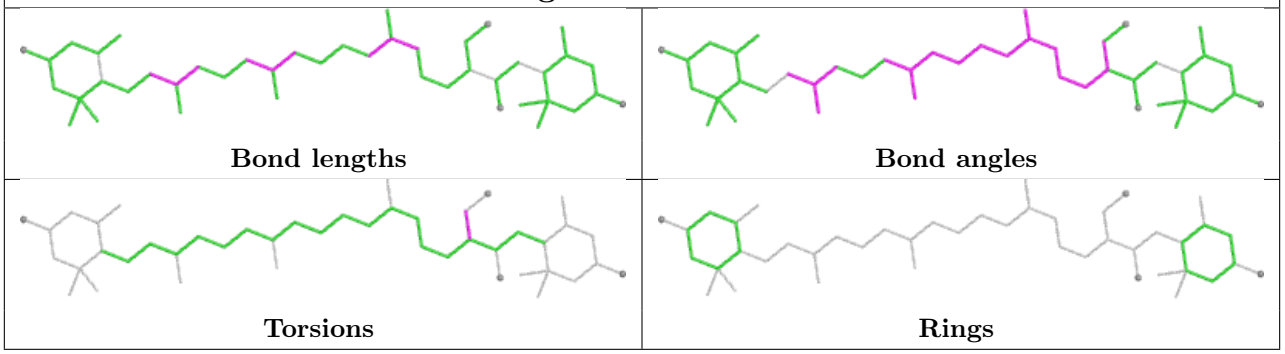


Torsions

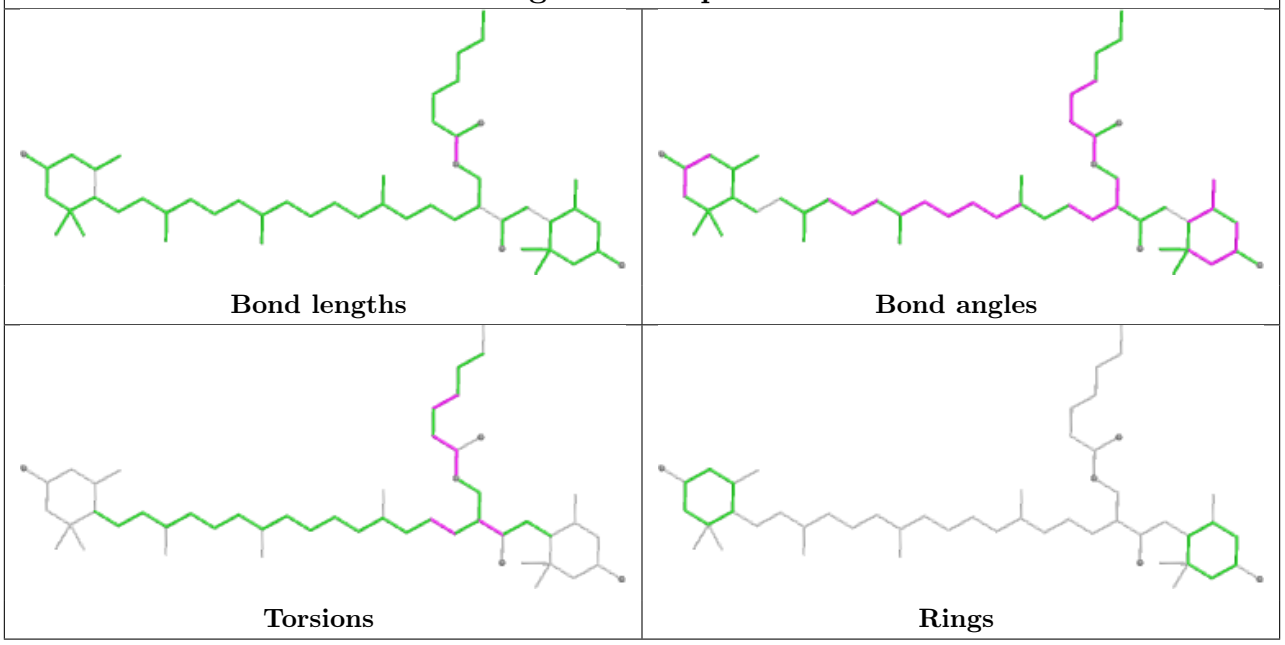


Rings

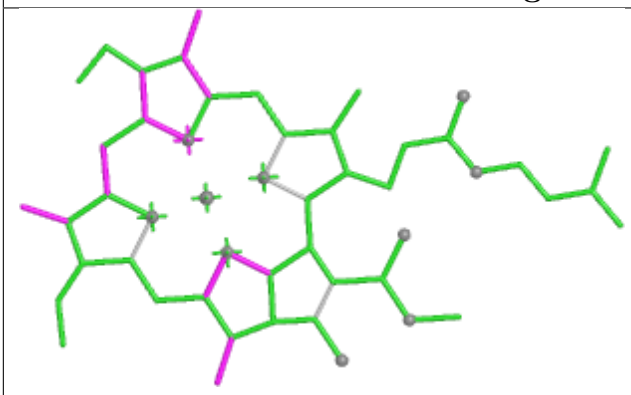
Ligand 0IE u 303



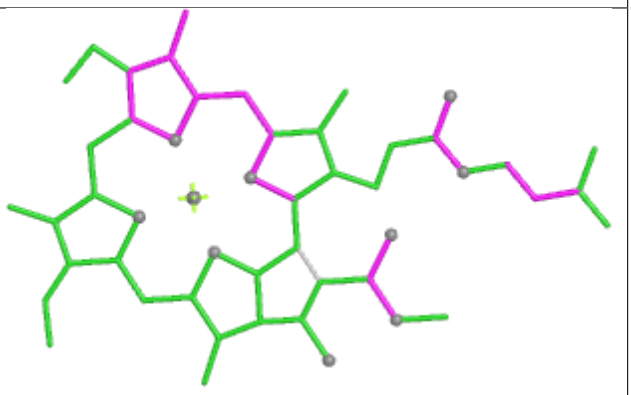
Ligand 0UR p 301



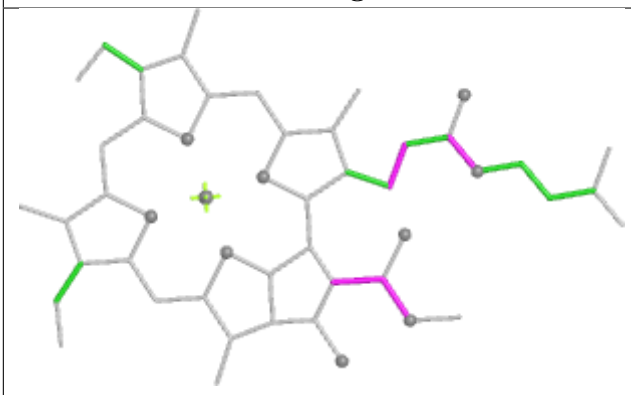
Ligand CLA Y 307



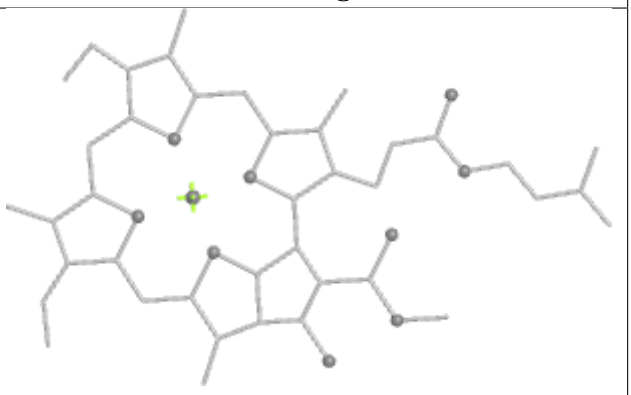
Bond lengths



Bond angles

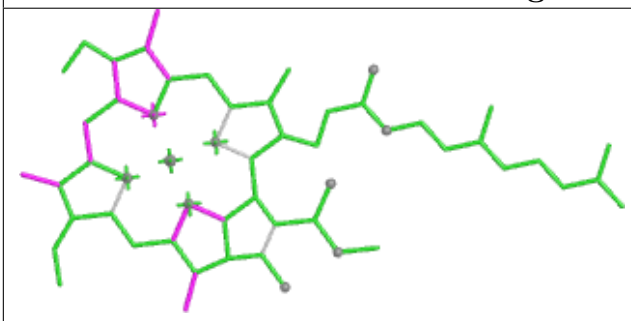


Torsions

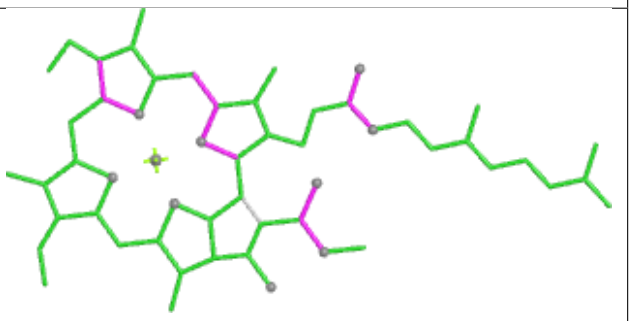


Rings

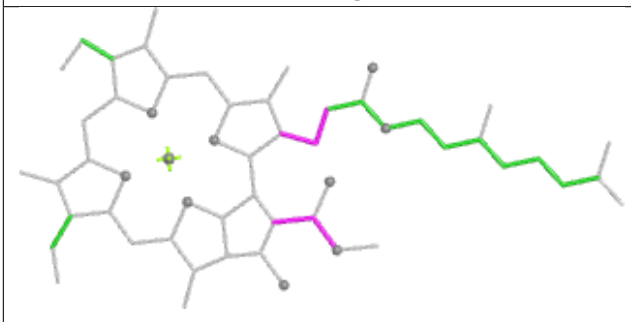
Ligand CLA S 609



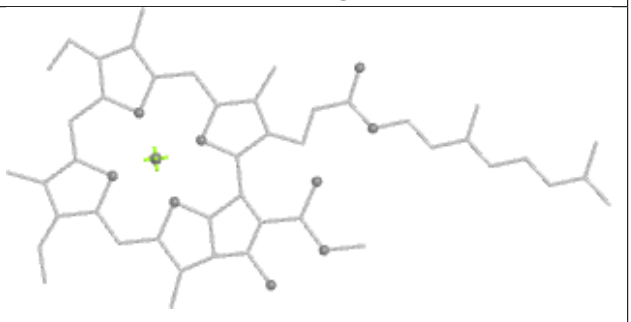
Bond lengths



Bond angles

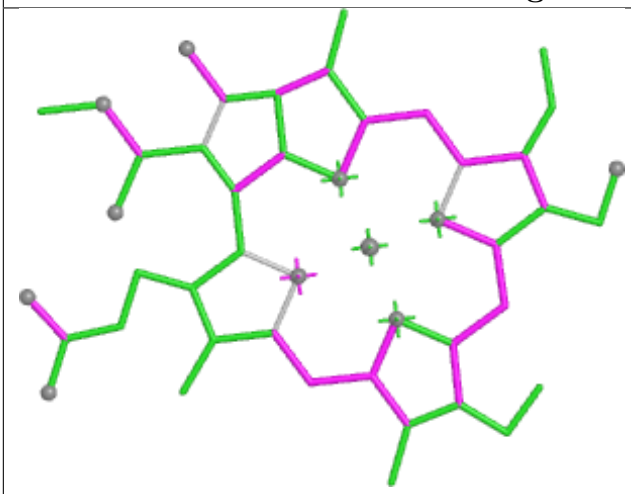


Torsions

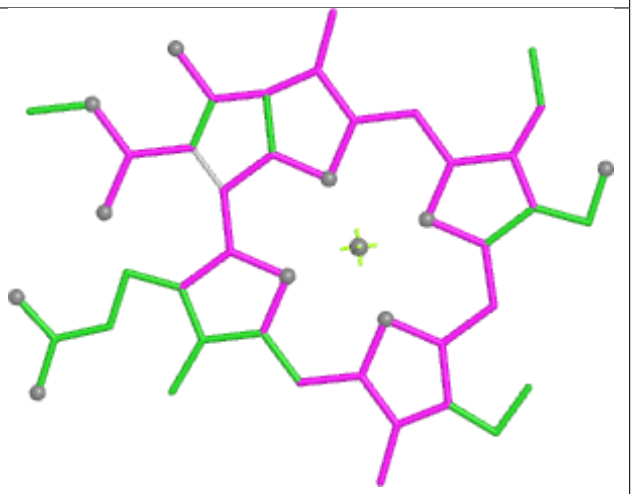


Rings

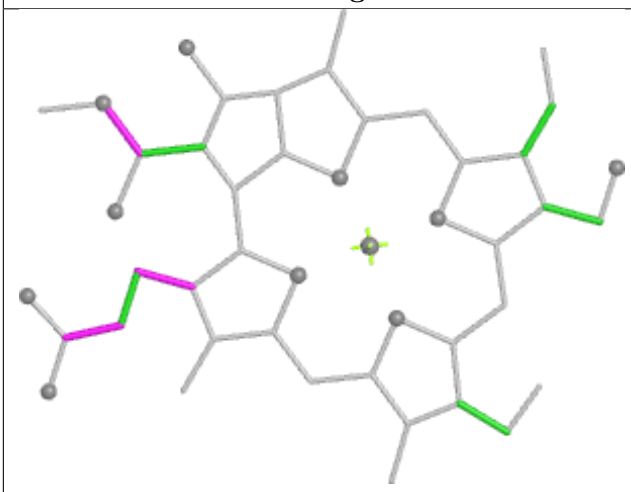
Ligand CHL S 606



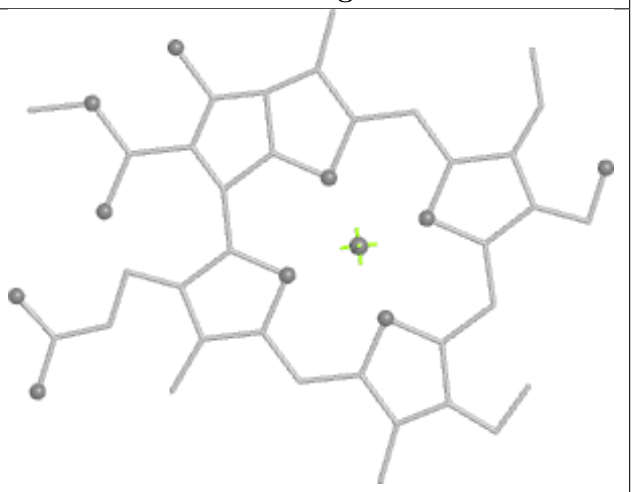
Bond lengths



Bond angles

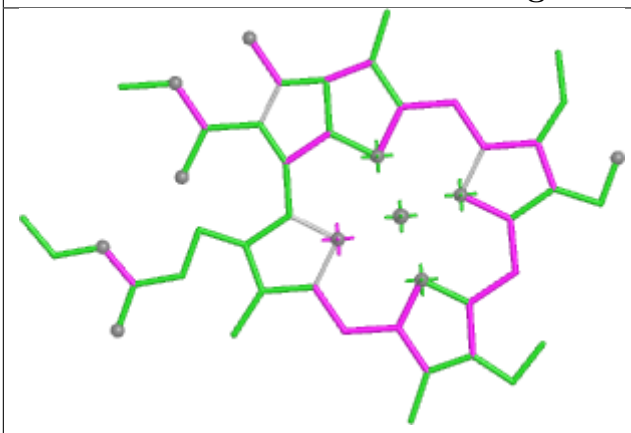


Torsions

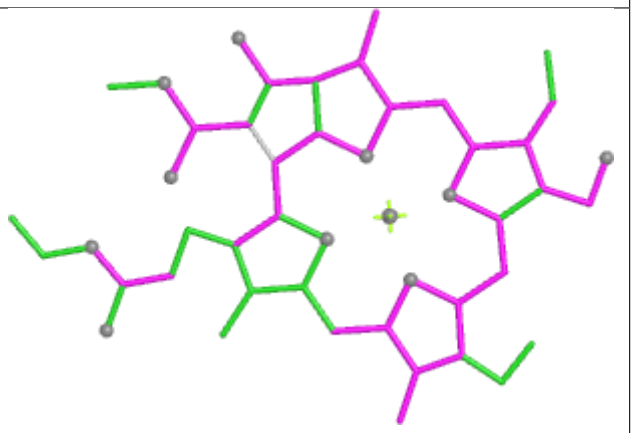


Rings

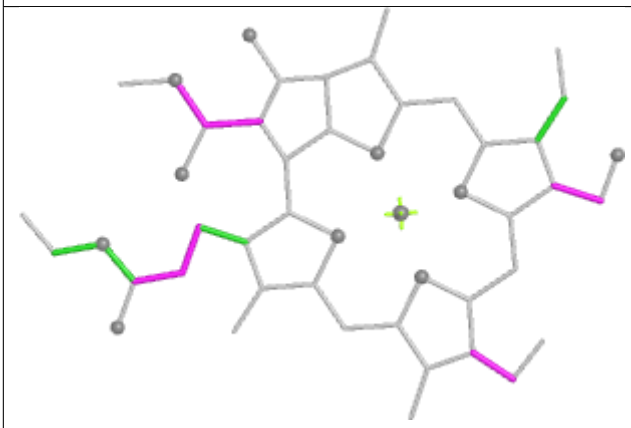
Ligand CHL 6 305



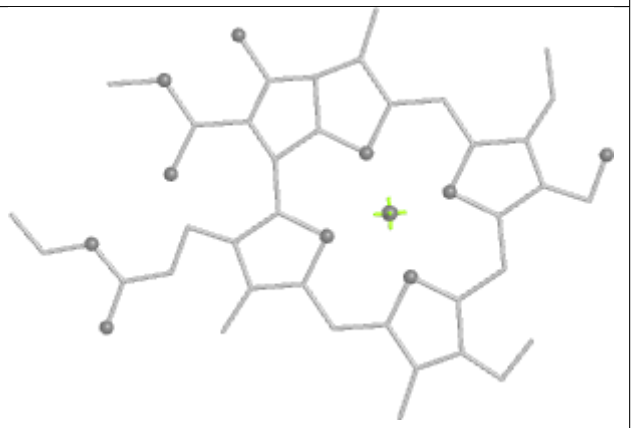
Bond lengths



Bond angles

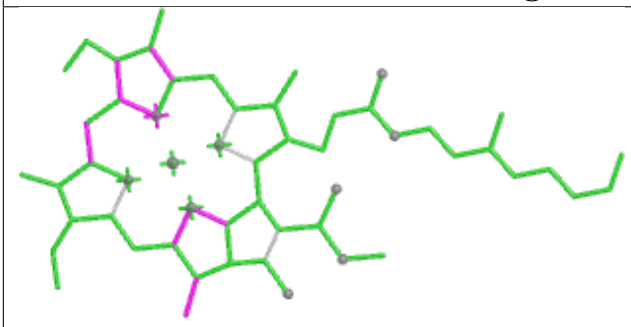


Torsions

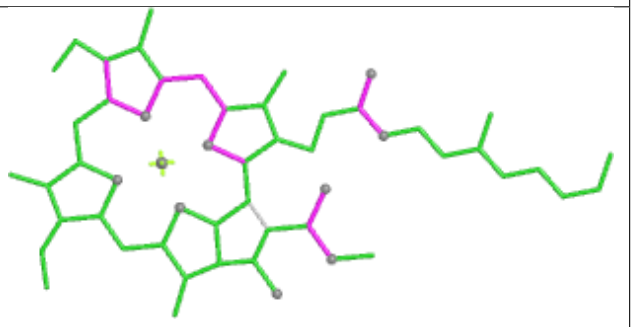


Rings

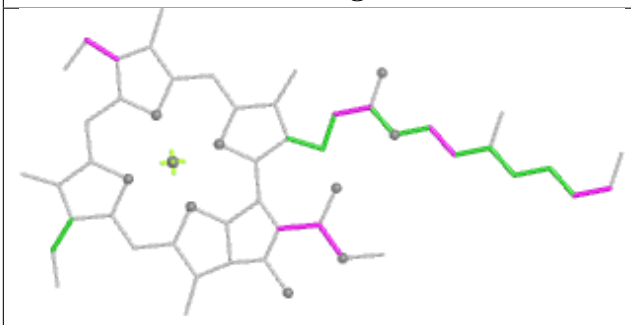
Ligand CLA N 306



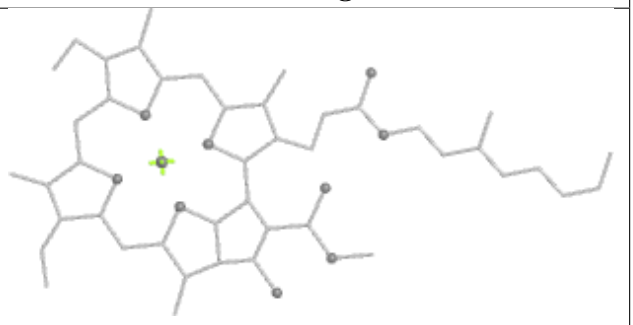
Bond lengths



Bond angles

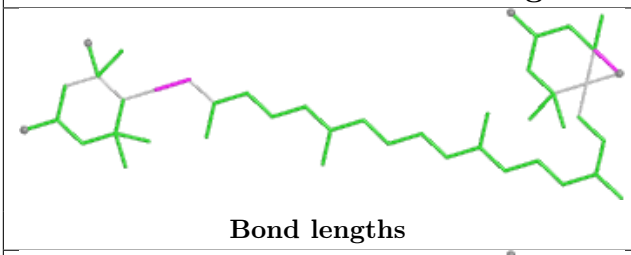


Torsions

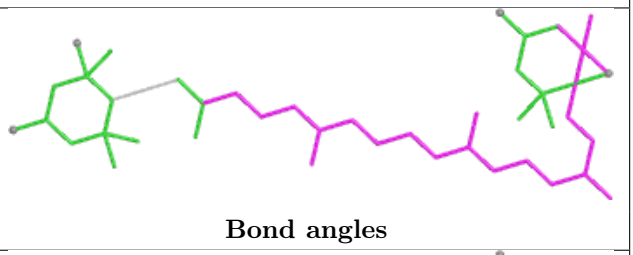


Rings

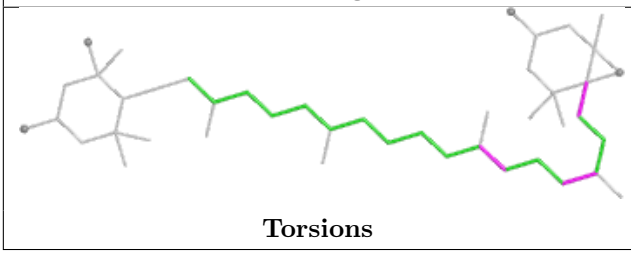
Ligand NEX S 617



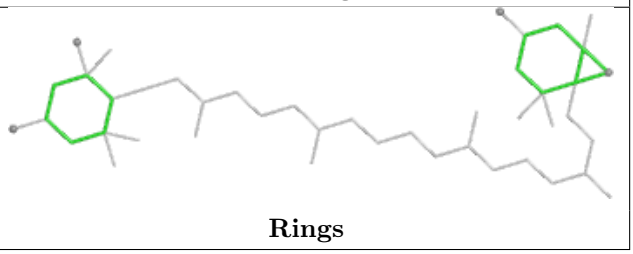
Bond lengths



Bond angles

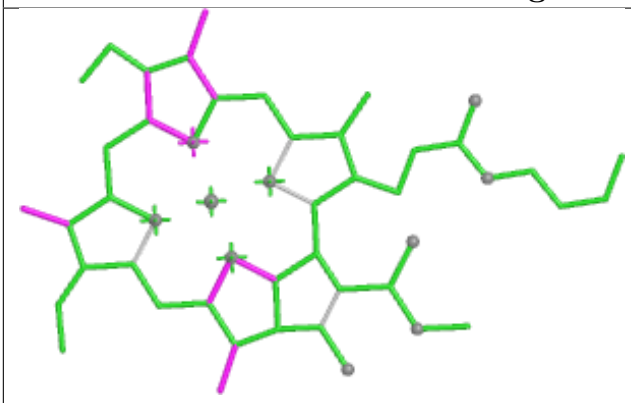


Torsions

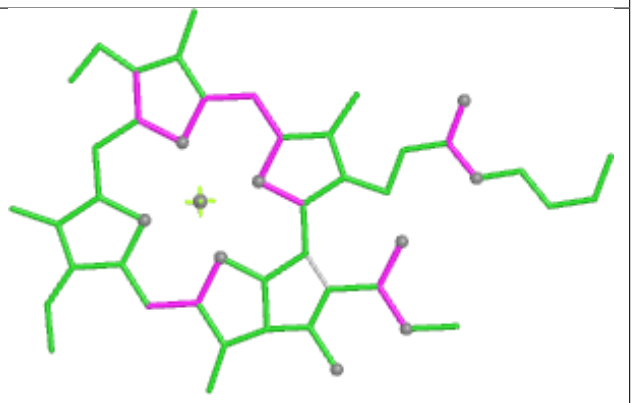


Rings

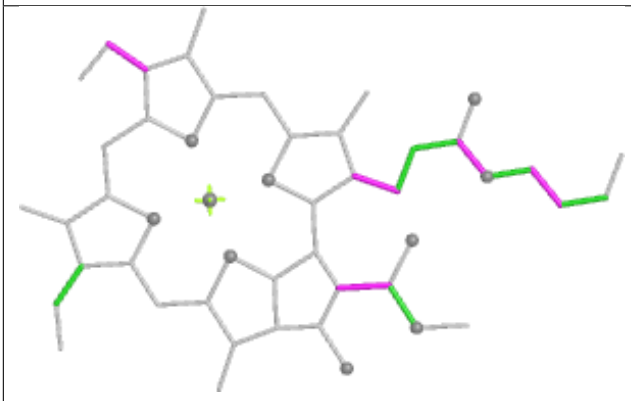
Ligand CLA a 605



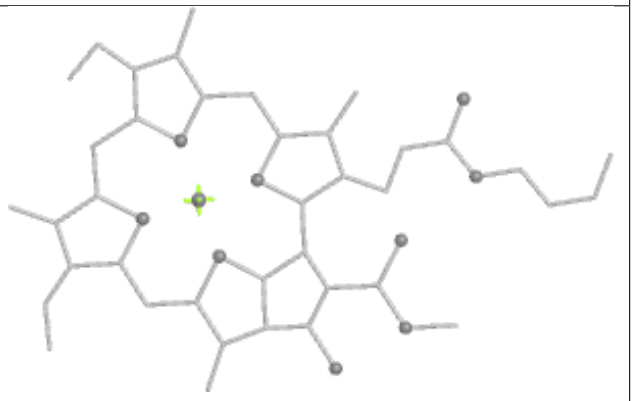
Bond lengths



Bond angles

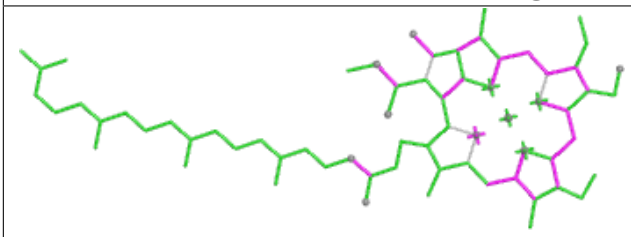


Torsions

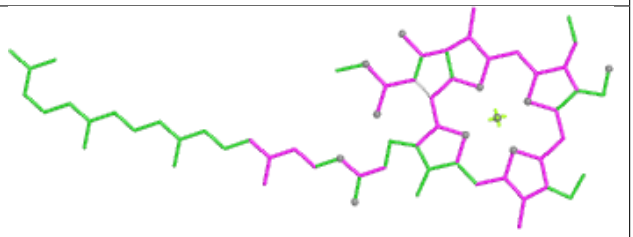


Rings

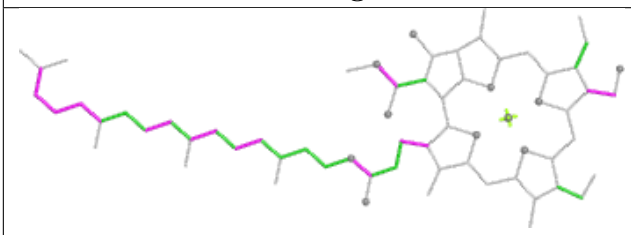
Ligand CHL 9 304



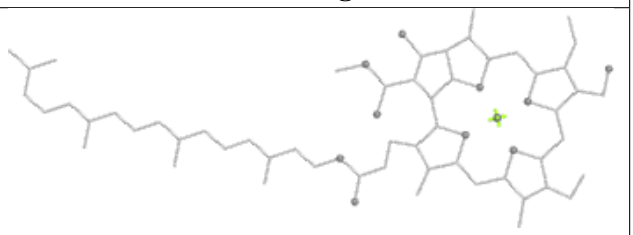
Bond lengths



Bond angles

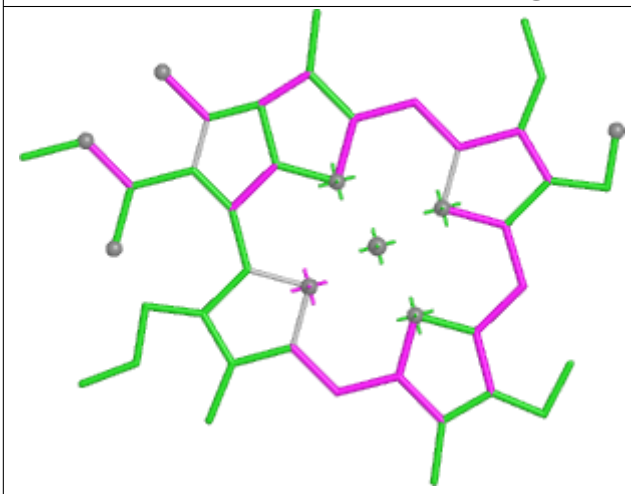


Torsions

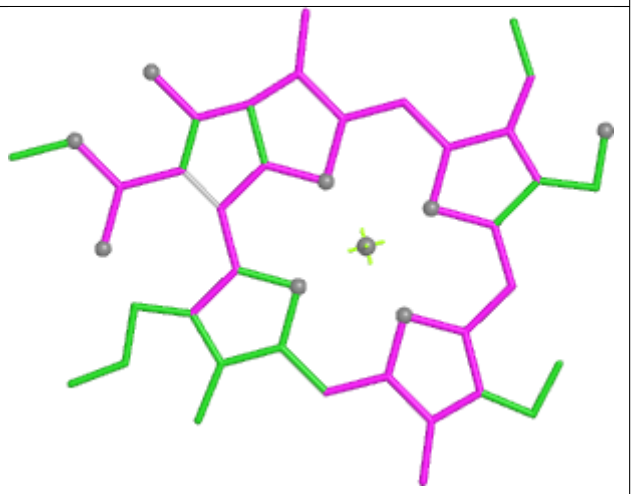


Rings

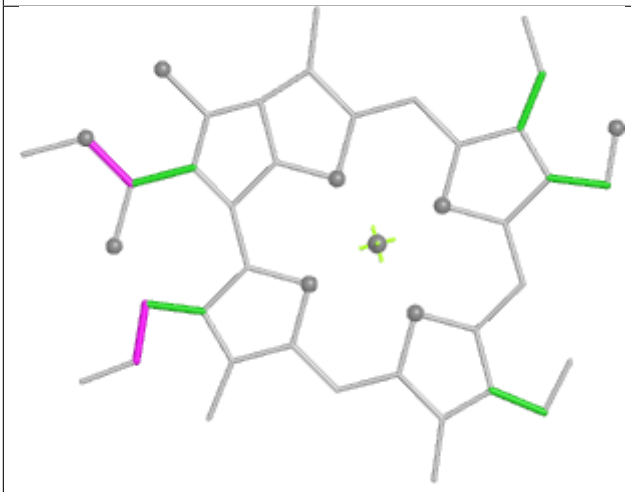
Ligand CHL 4 311



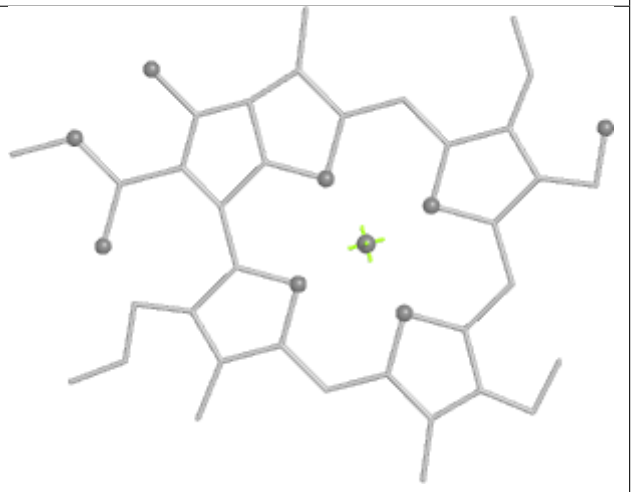
Bond lengths



Bond angles

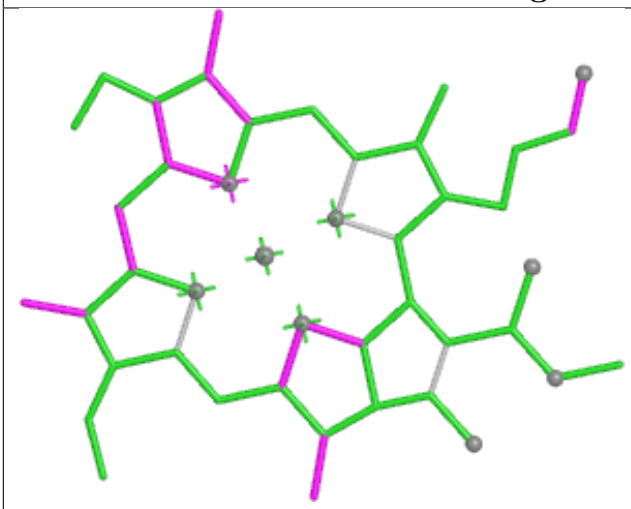


Torsions

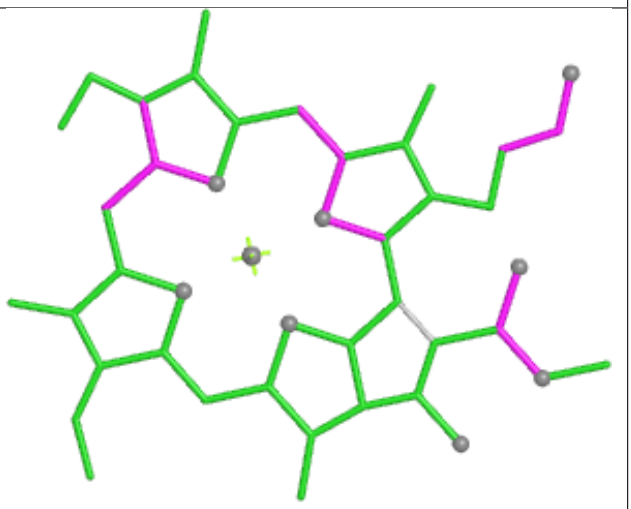


Rings

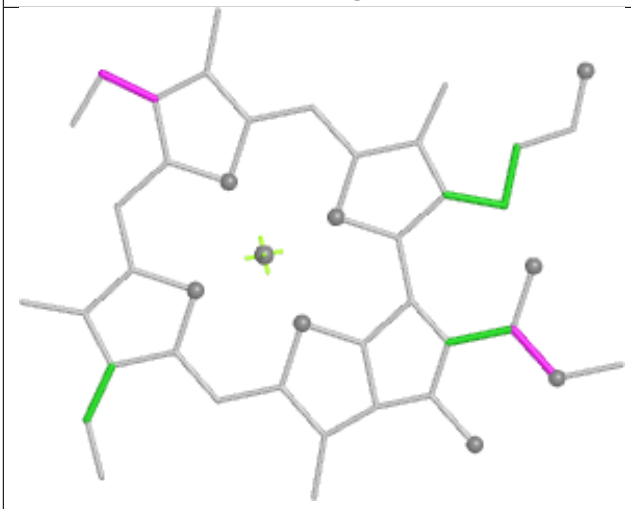
Ligand CLA s 411



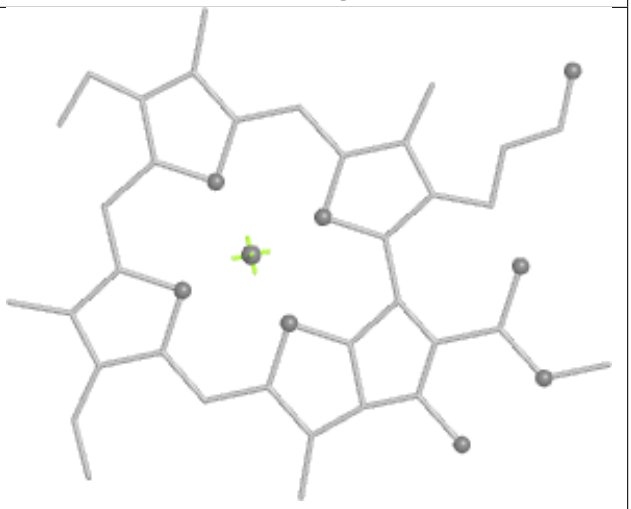
Bond lengths



Bond angles

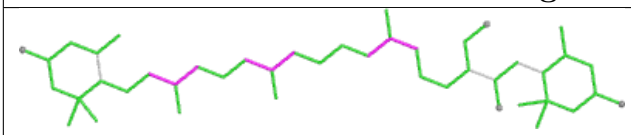


Torsions

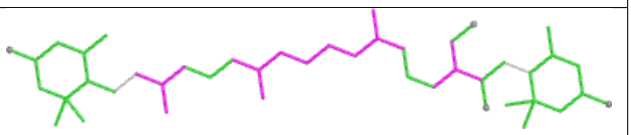


Rings

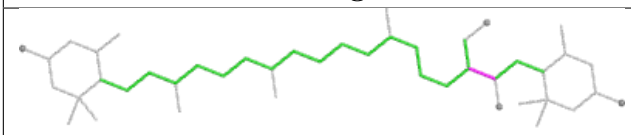
Ligand 0IE r 315



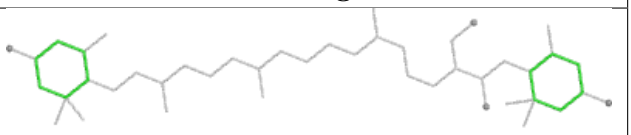
Bond lengths



Bond angles

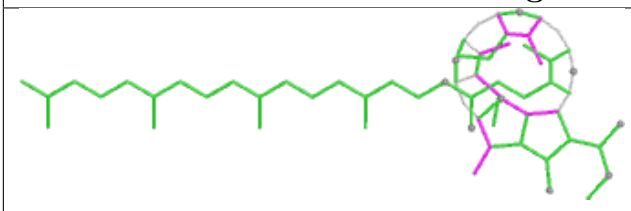


Torsions

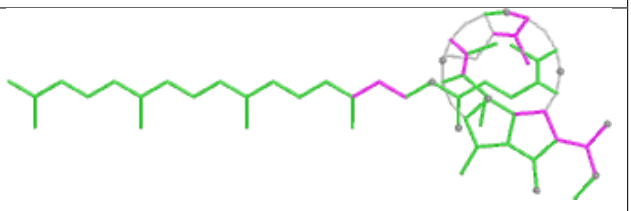


Rings

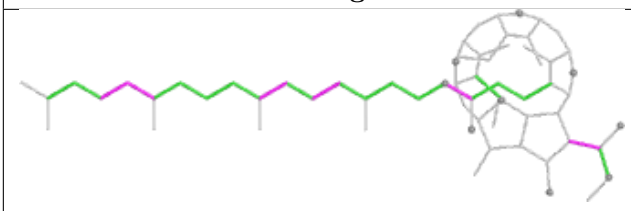
Ligand PHO a 606



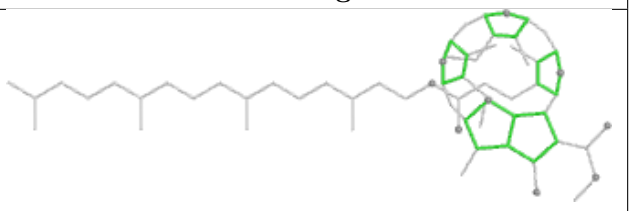
Bond lengths



Bond angles

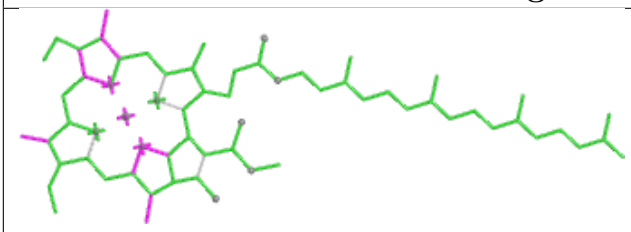


Torsions

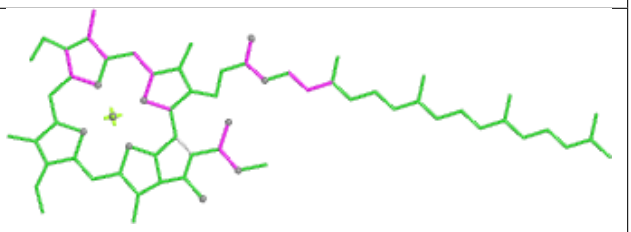


Rings

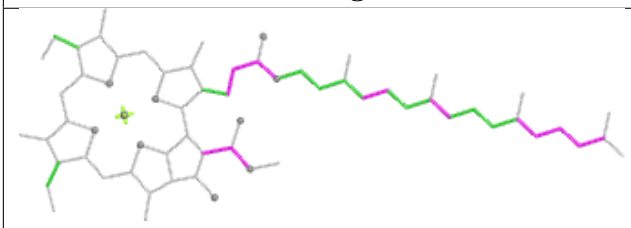
Ligand CLA b 606



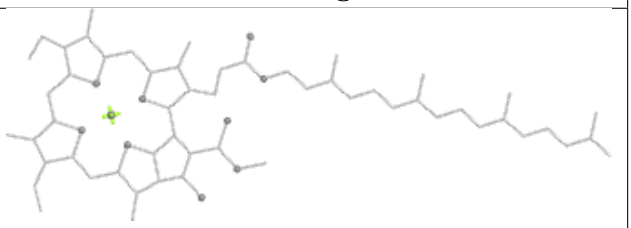
Bond lengths



Bond angles

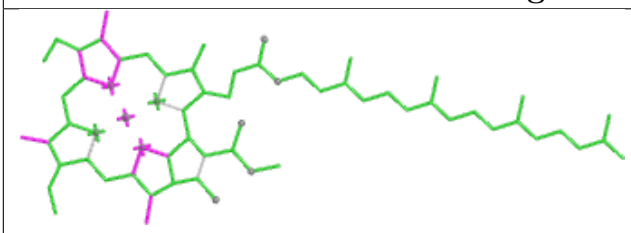


Torsions

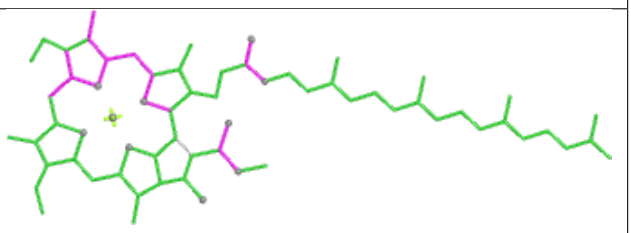


Rings

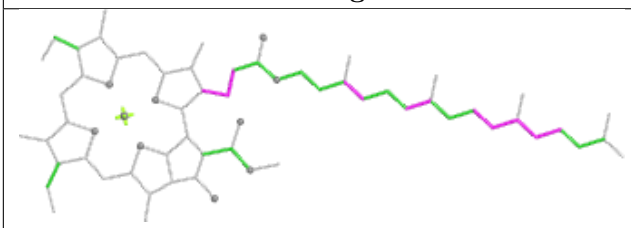
Ligand CLA b 603



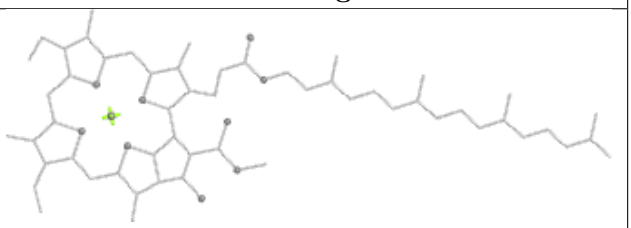
Bond lengths



Bond angles

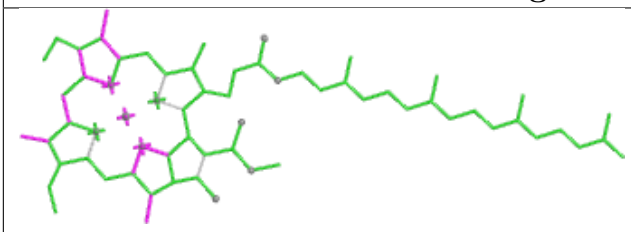


Torsions

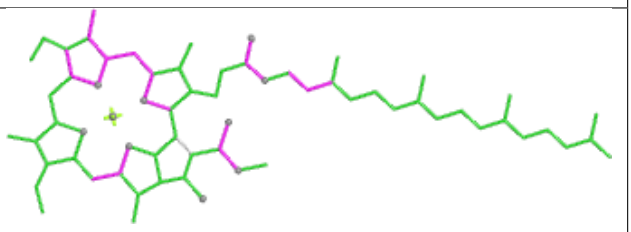


Rings

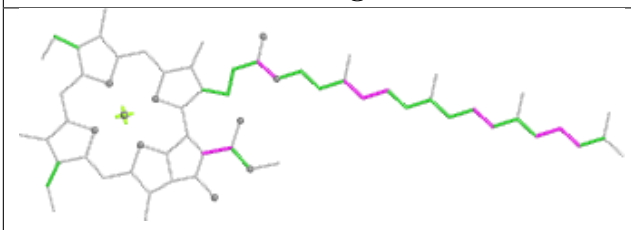
Ligand CLA c 610



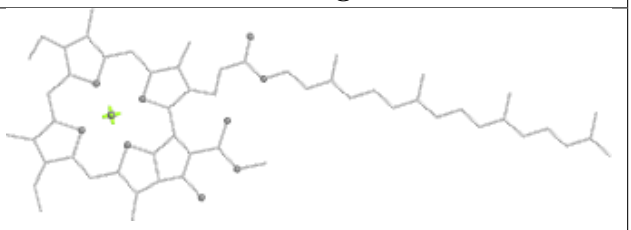
Bond lengths



Bond angles

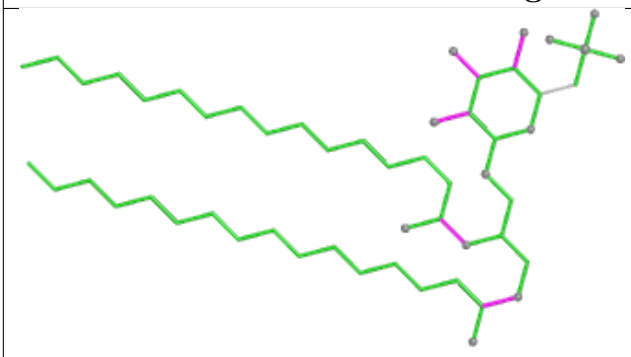


Torsions

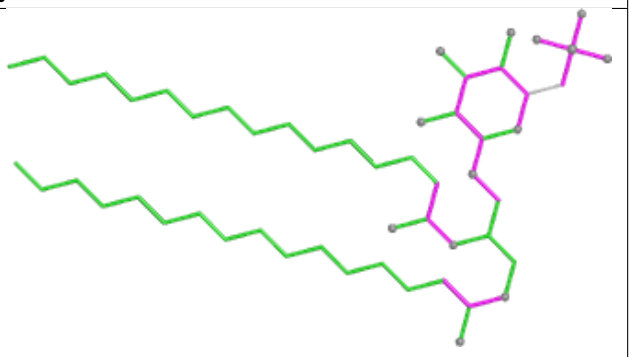


Rings

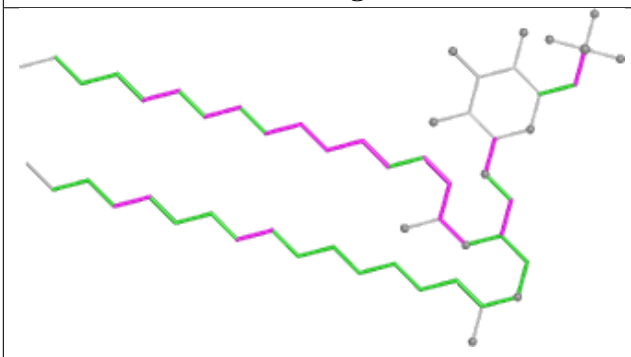
Ligand SQD B 618



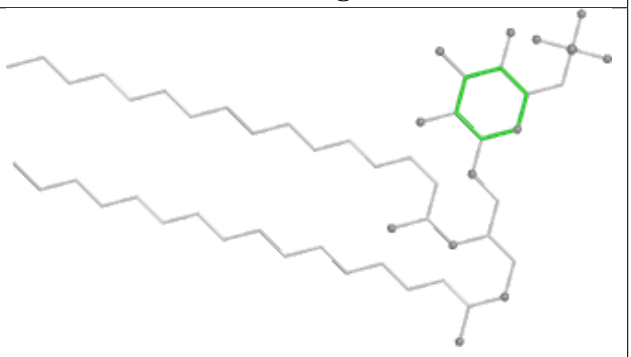
Bond lengths



Bond angles

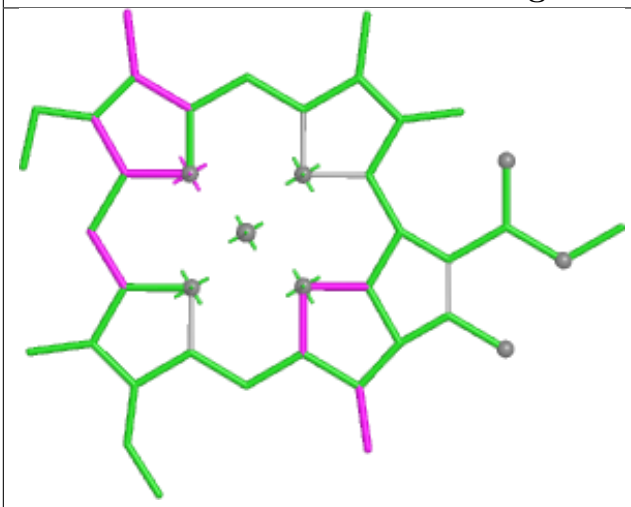


Torsions

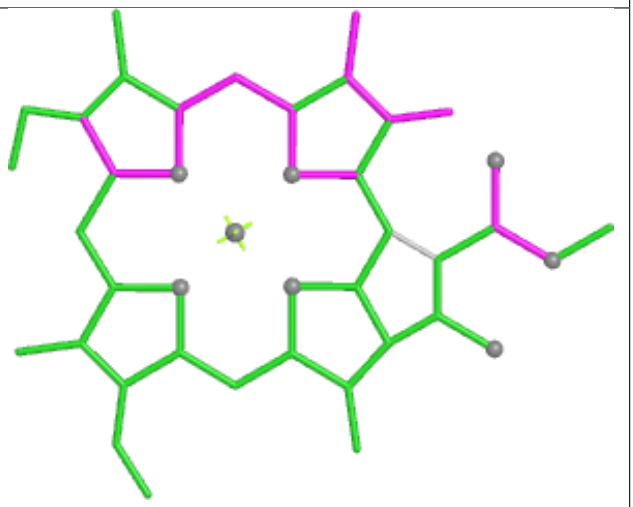


Rings

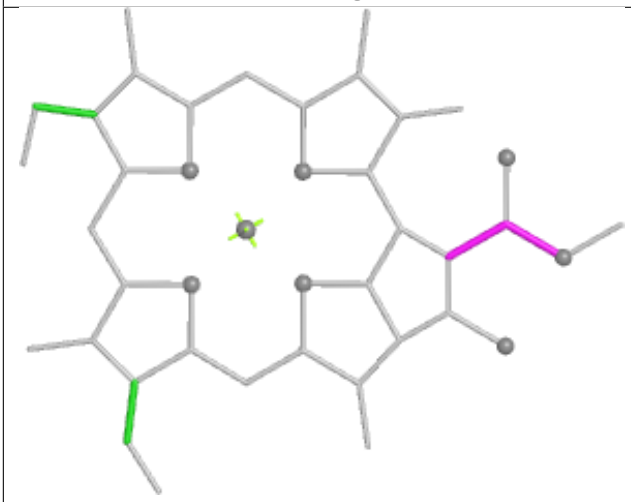
Ligand CLA 4 307



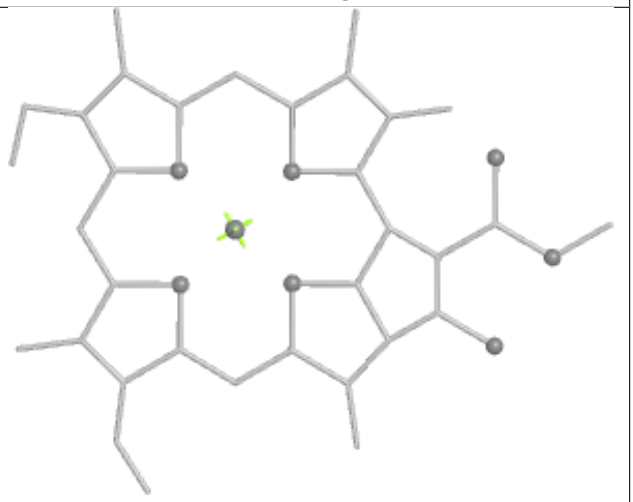
Bond lengths



Bond angles

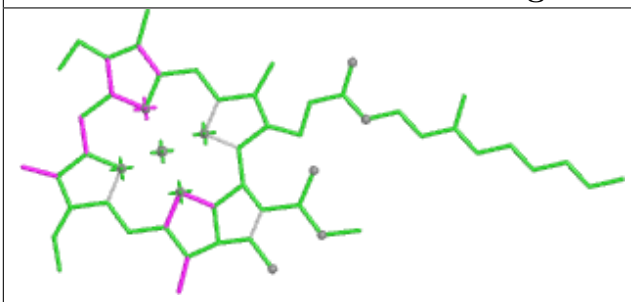


Torsions

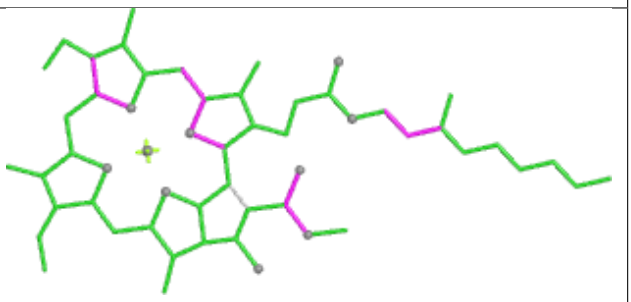


Rings

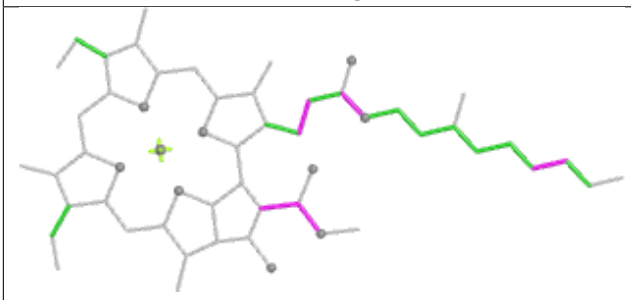
Ligand CLA u 317



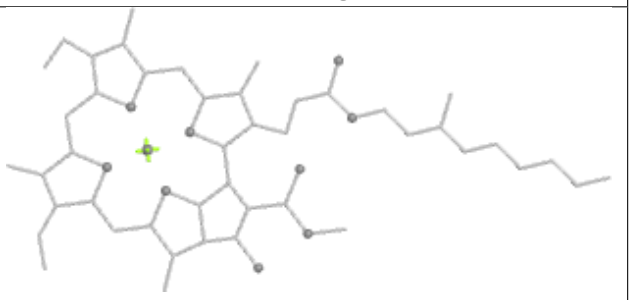
Bond lengths



Bond angles

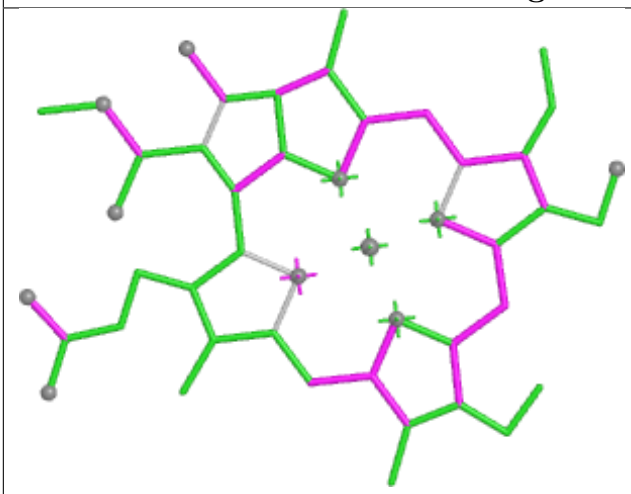


Torsions

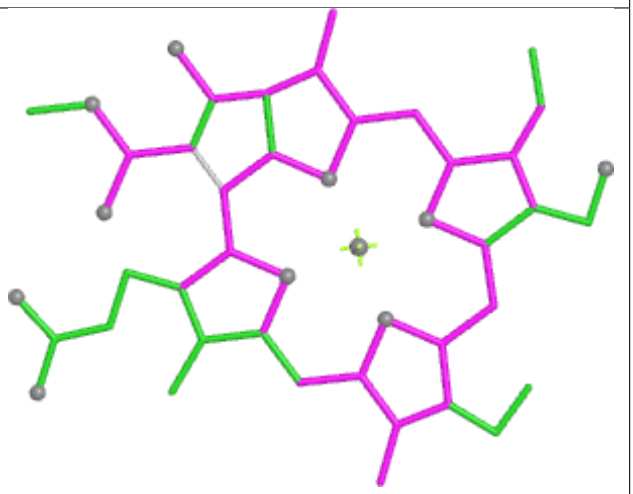


Rings

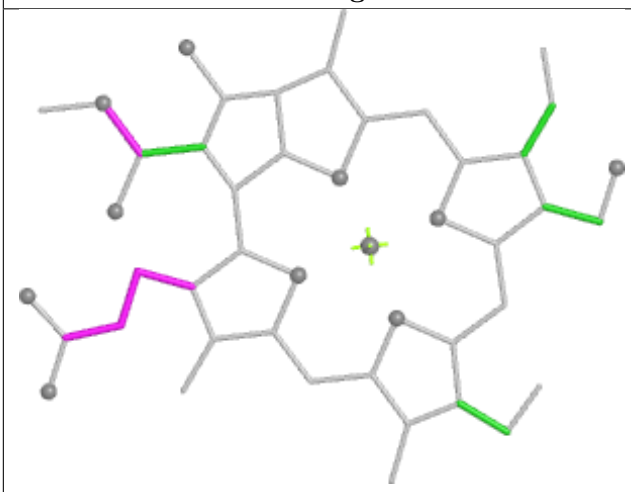
Ligand CHL 3 310



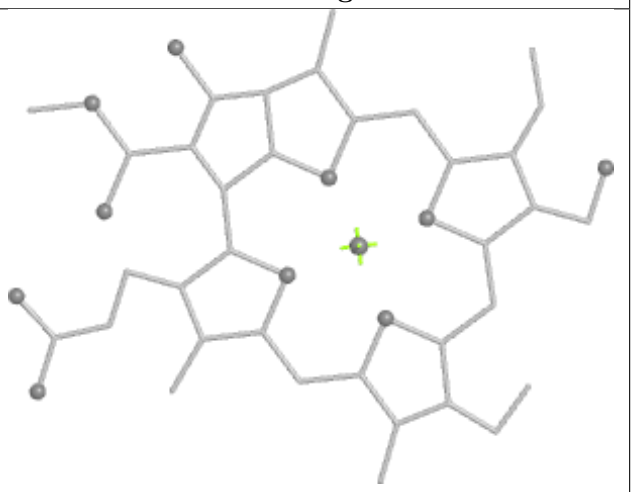
Bond lengths



Bond angles

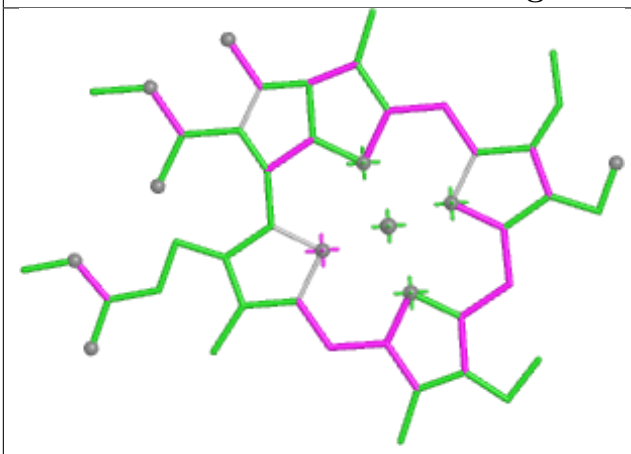


Torsions

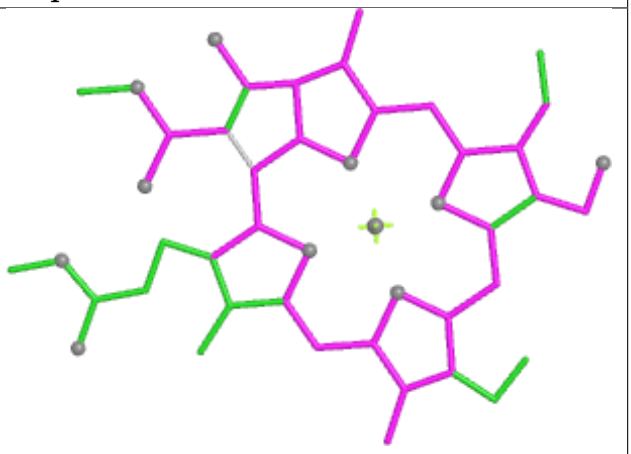


Rings

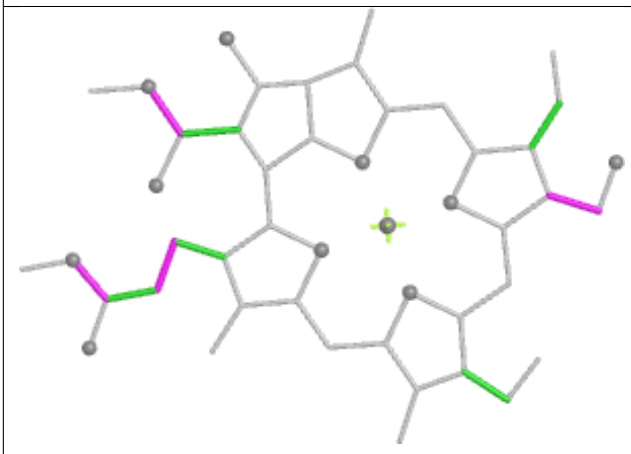
Ligand CHL p 312



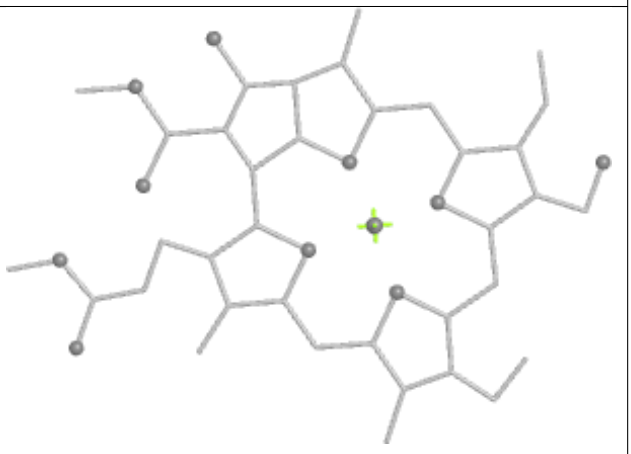
Bond lengths



Bond angles

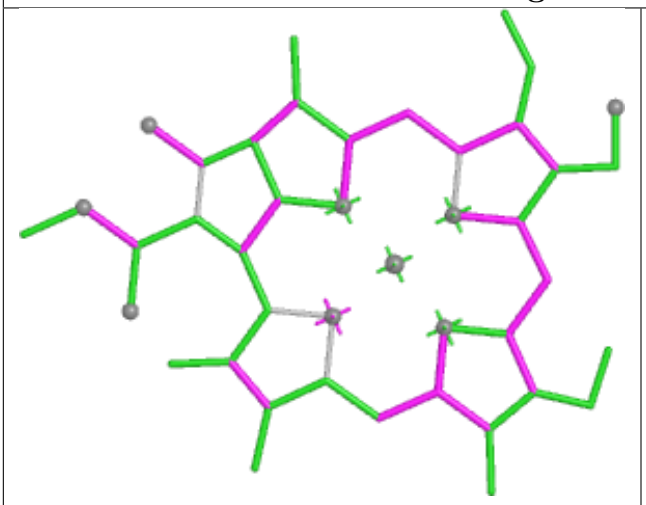


Torsions

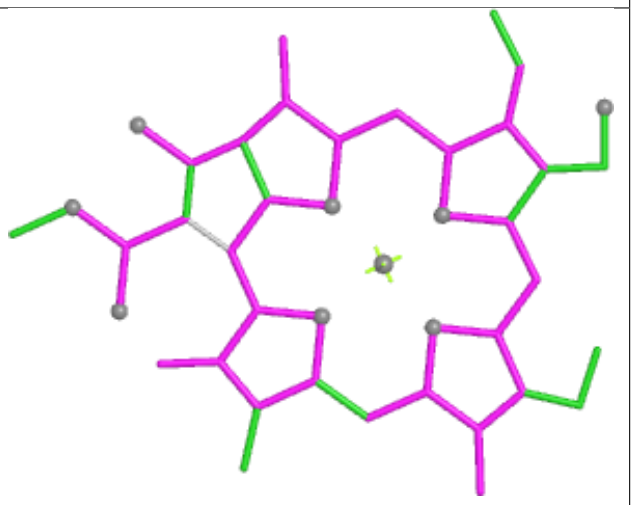


Rings

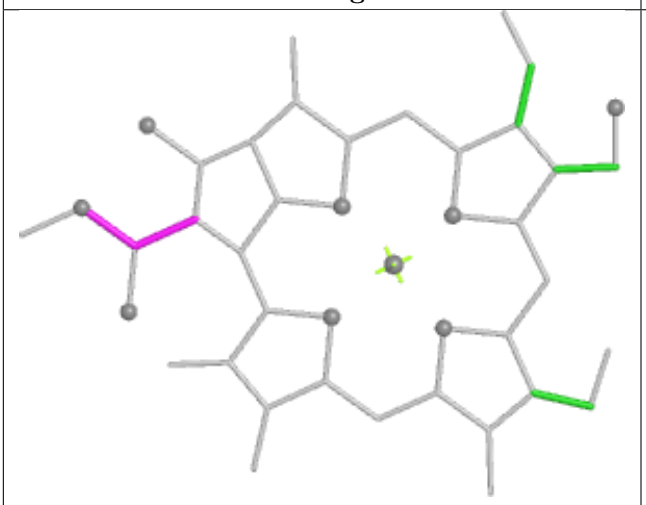
Ligand CHL 7 318



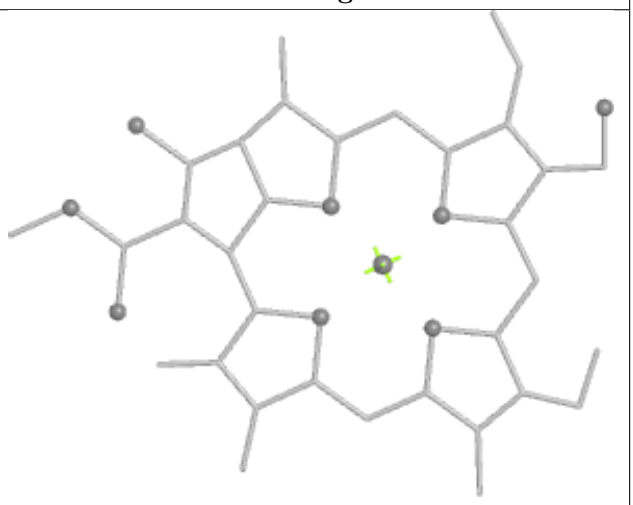
Bond lengths



Bond angles

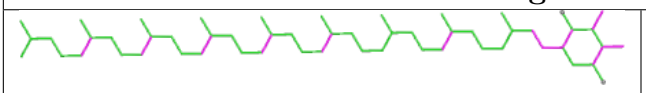


Torsions

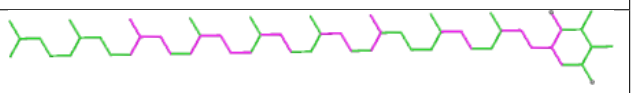


Rings

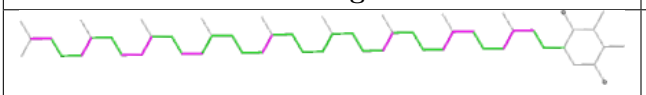
Ligand PL9 D 406



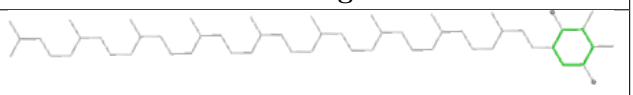
Bond lengths



Bond angles

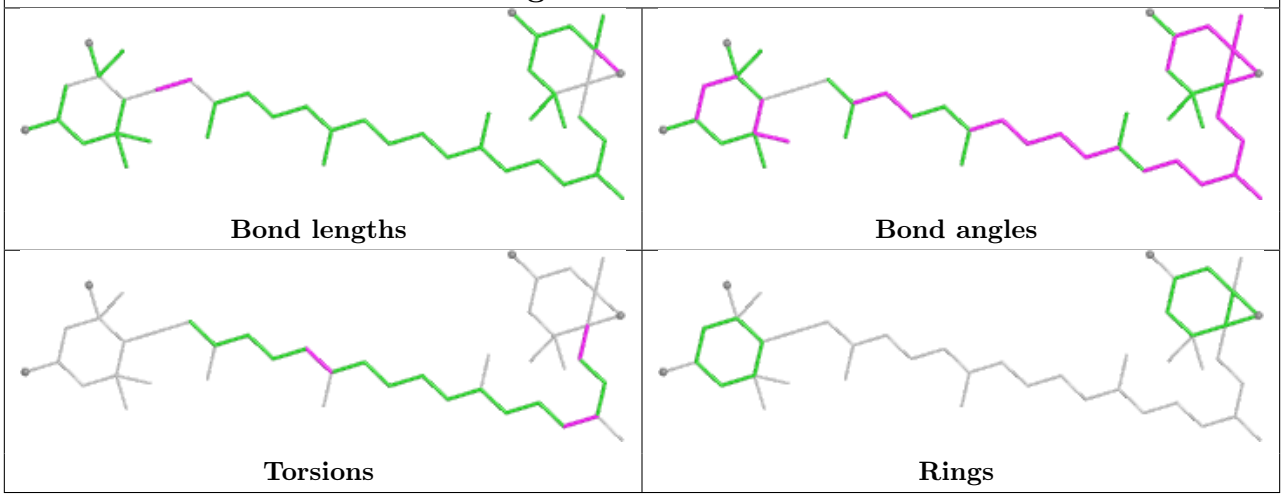


Torsions

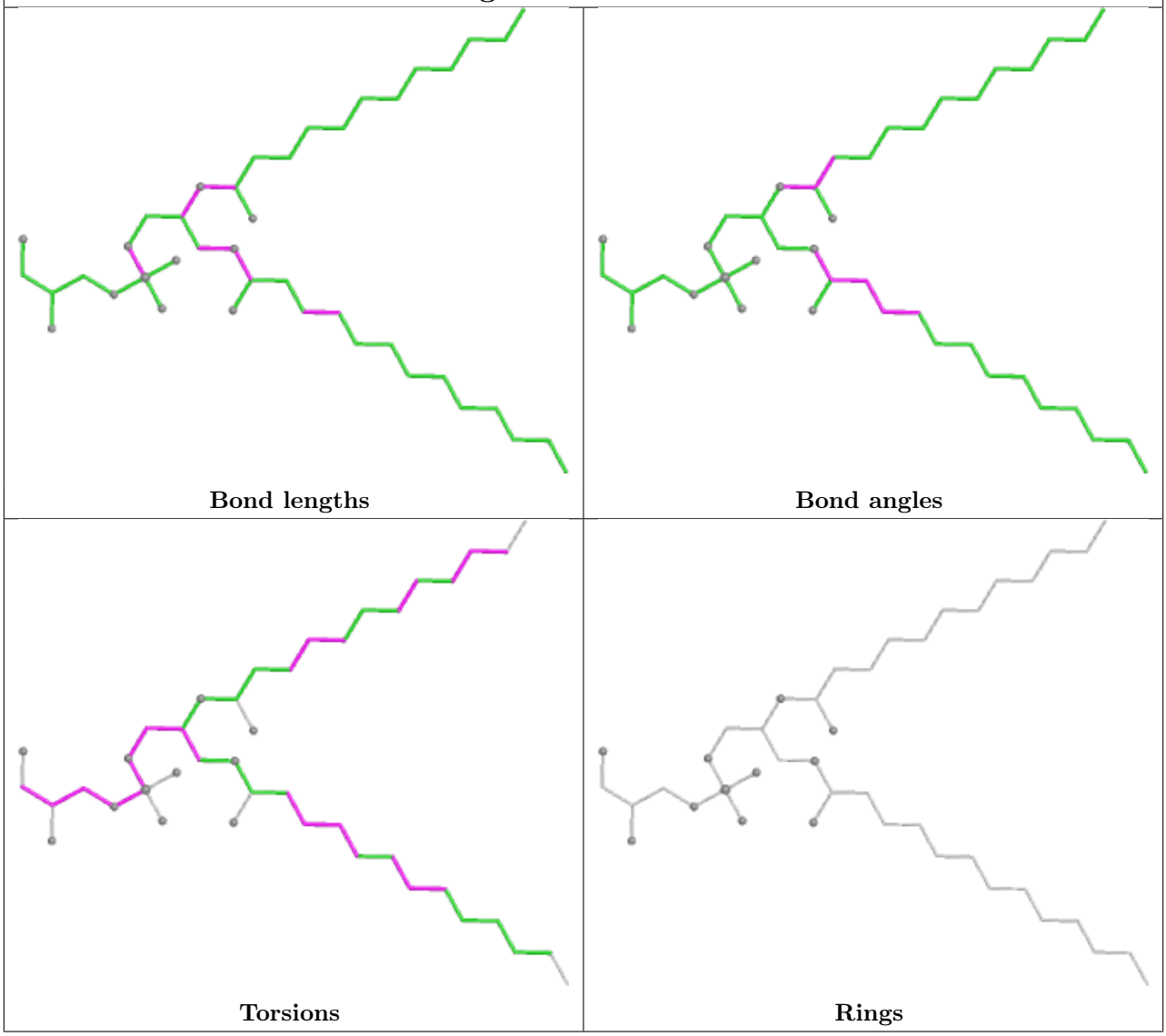


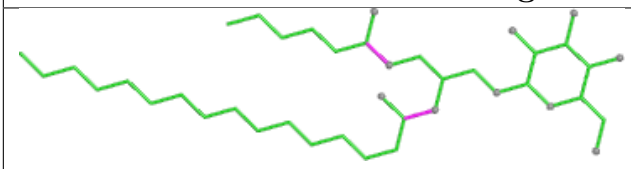
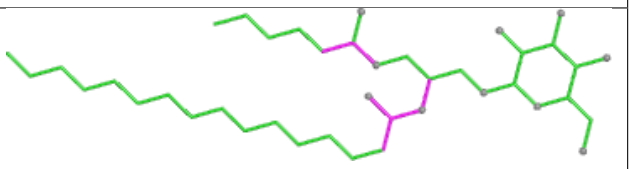
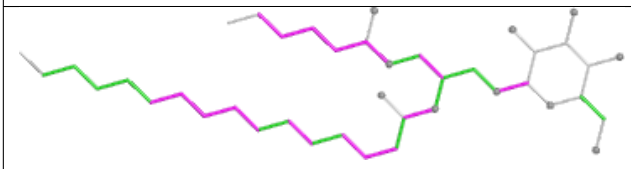
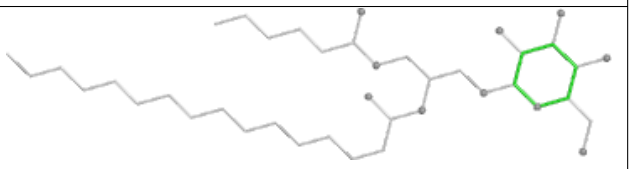
Rings

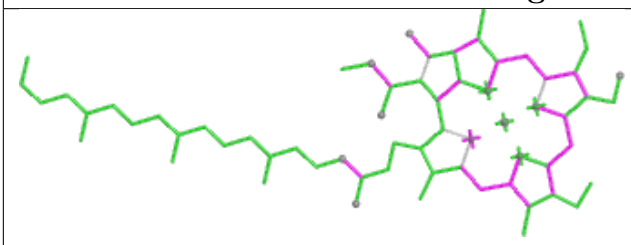
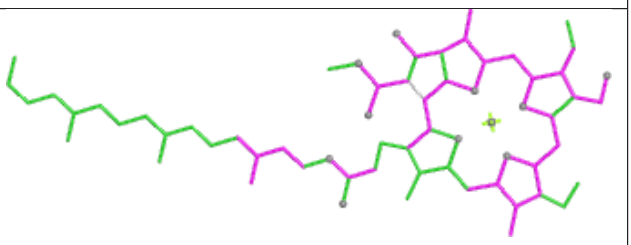
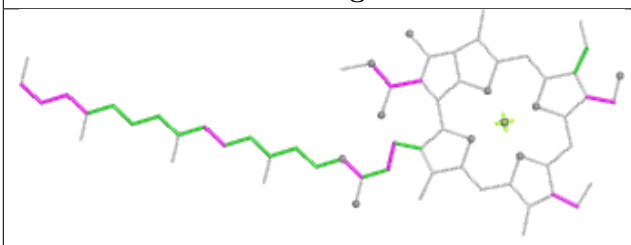
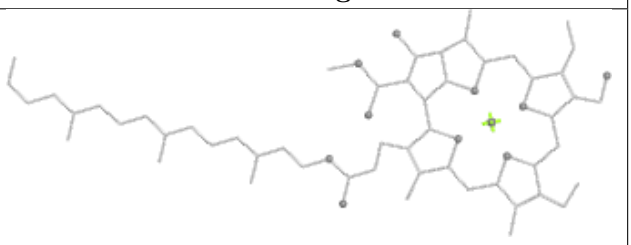
Ligand NEX 6 303



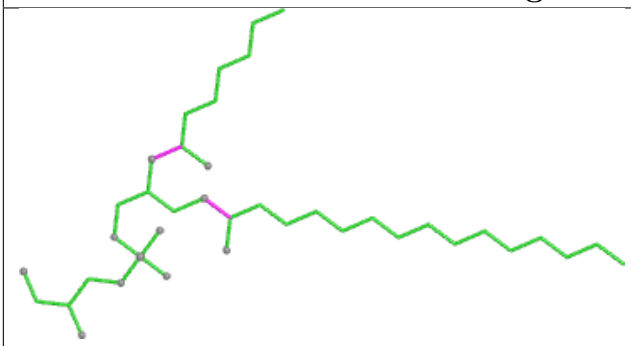
Ligand LHG 1 318



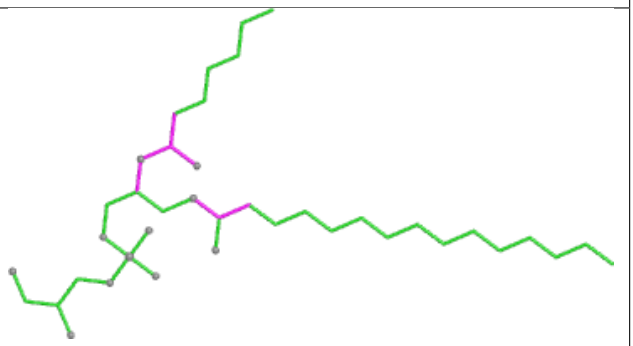
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 9 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

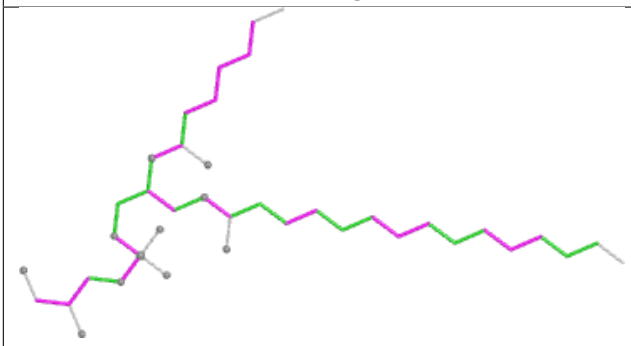
Ligand LHG d 408



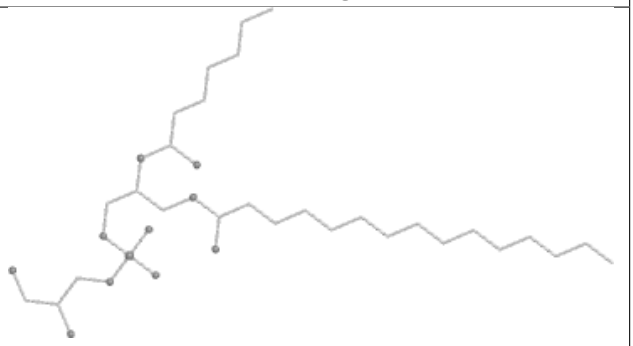
Bond lengths



Bond angles

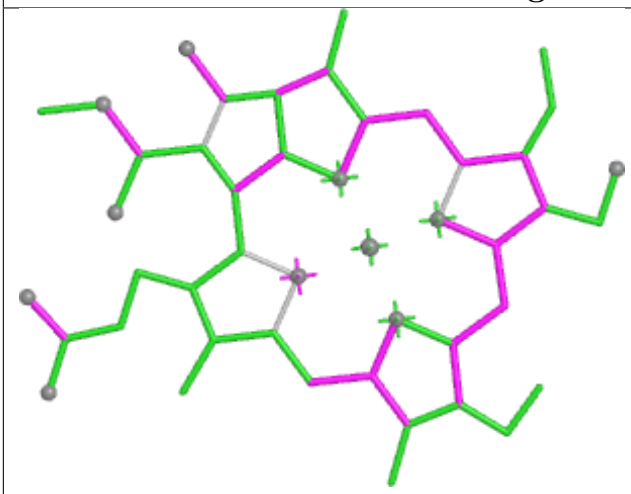


Torsions

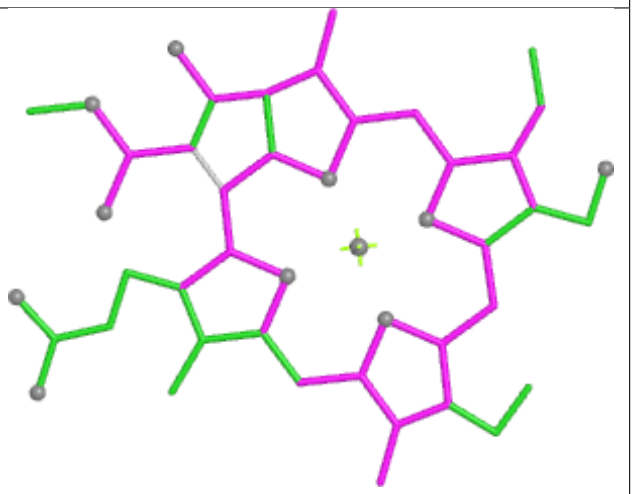


Rings

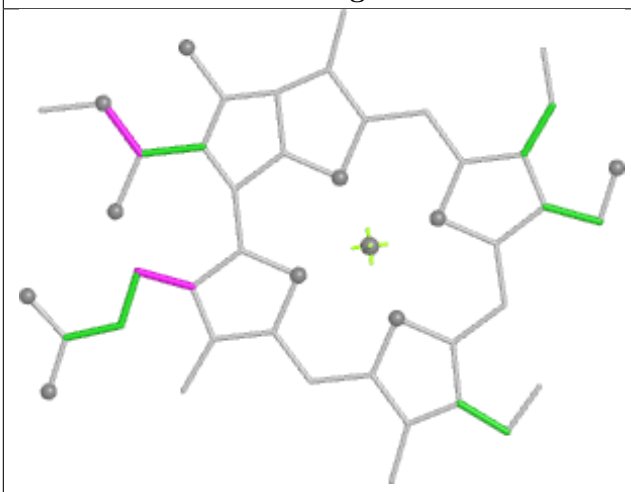
Ligand CHL 9 310



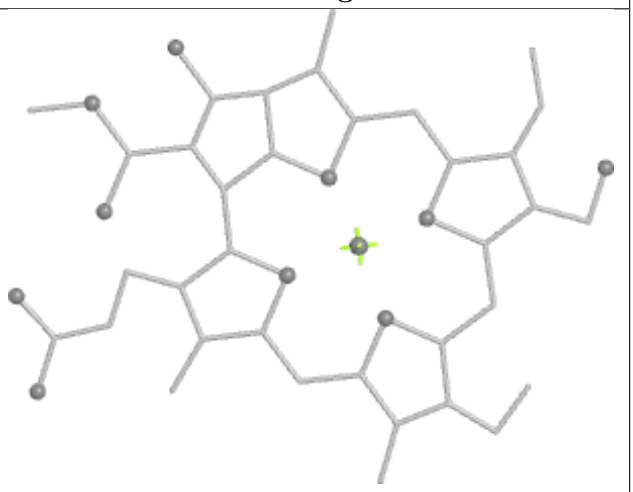
Bond lengths



Bond angles

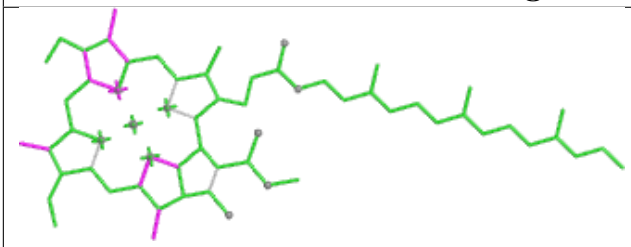


Torsions

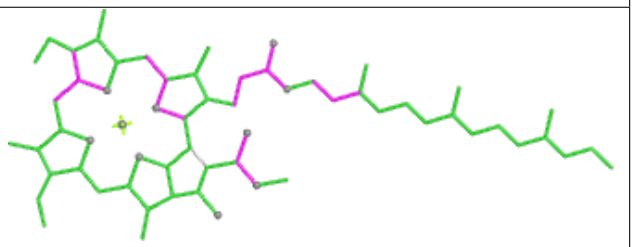


Rings

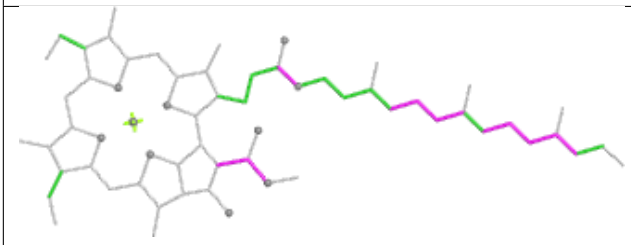
Ligand CLA B 604



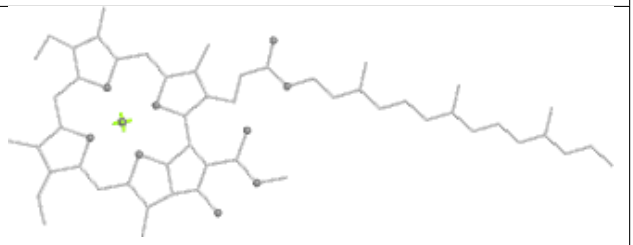
Bond lengths



Bond angles

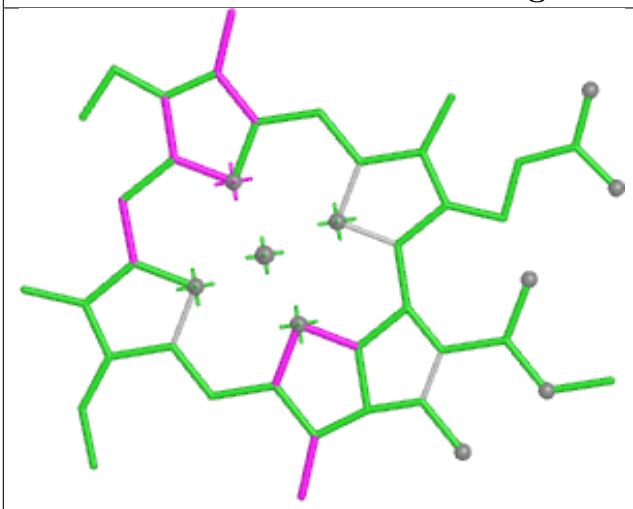


Torsions

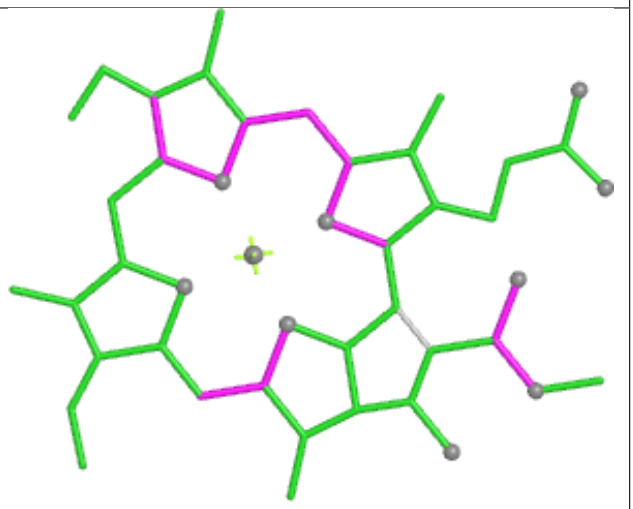


Rings

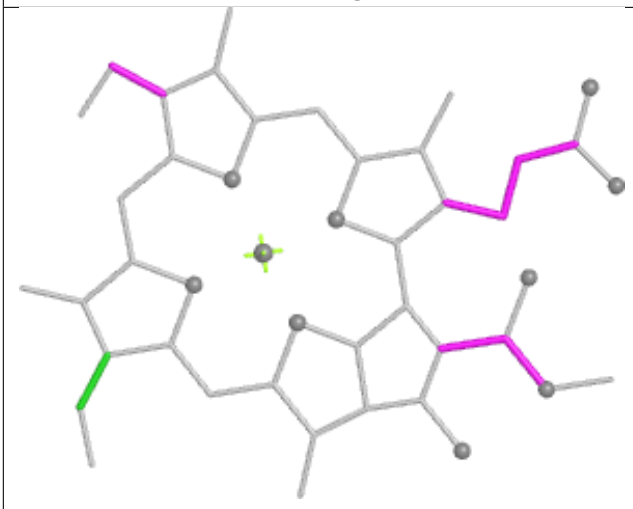
Ligand CLA 6 316



Bond lengths



Bond angles

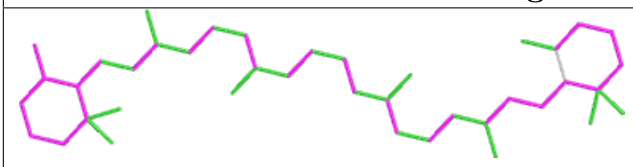


Torsions

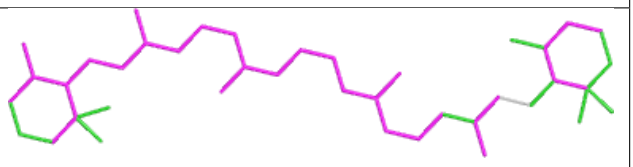


Rings

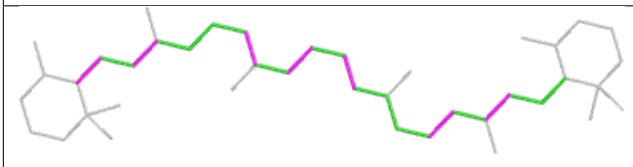
Ligand 8CT X 601



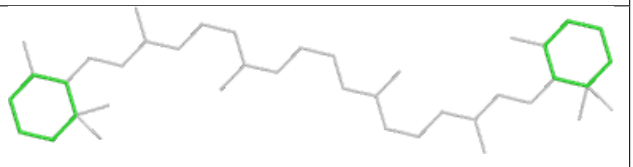
Bond lengths



Bond angles

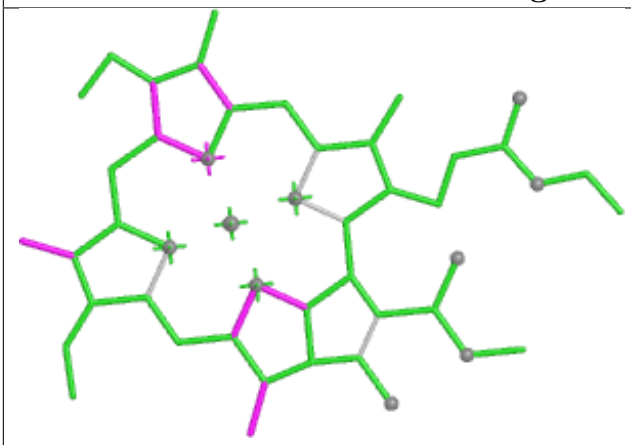


Torsions

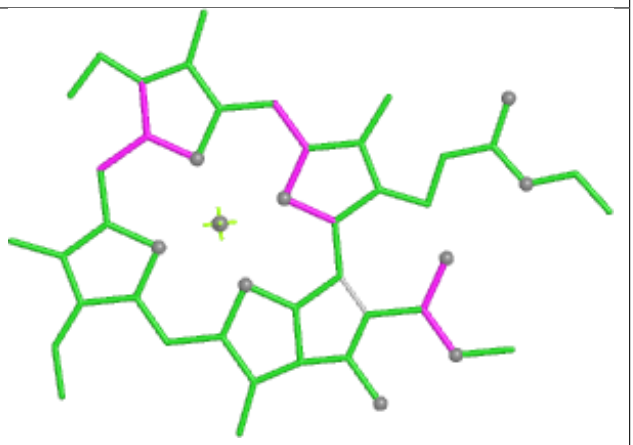


Rings

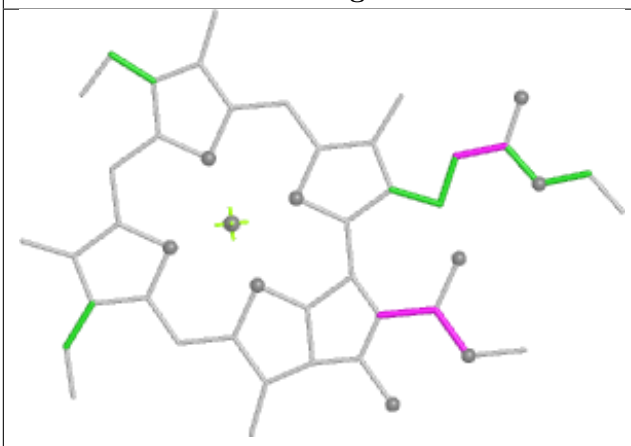
Ligand CLA r 304



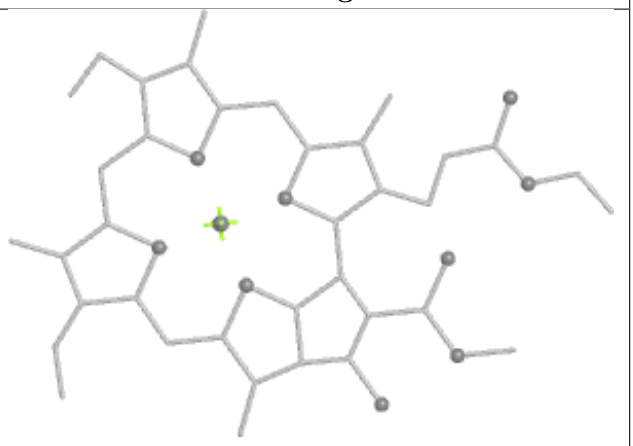
Bond lengths



Bond angles

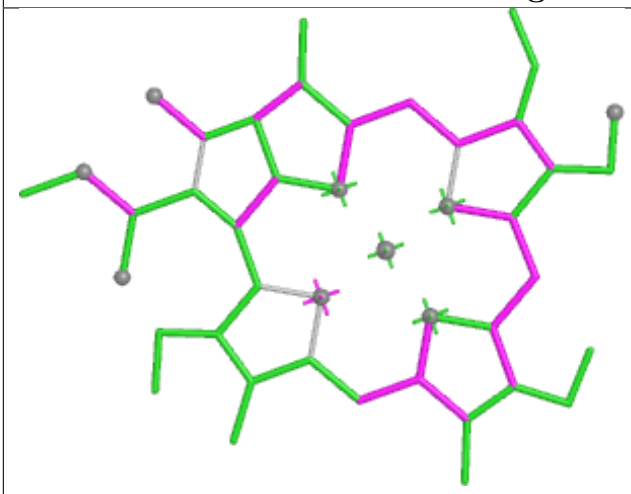


Torsions

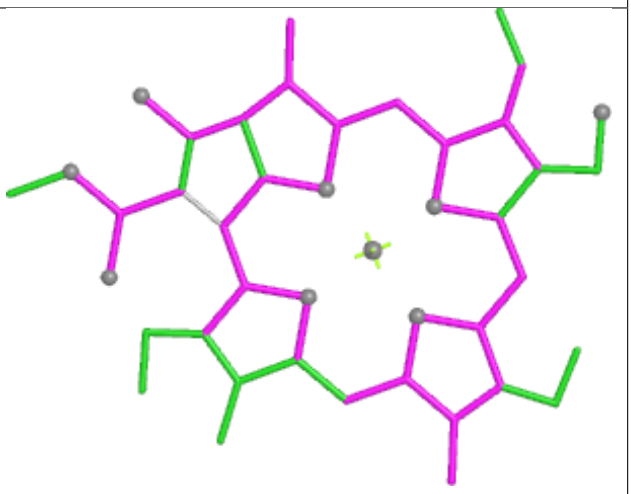


Rings

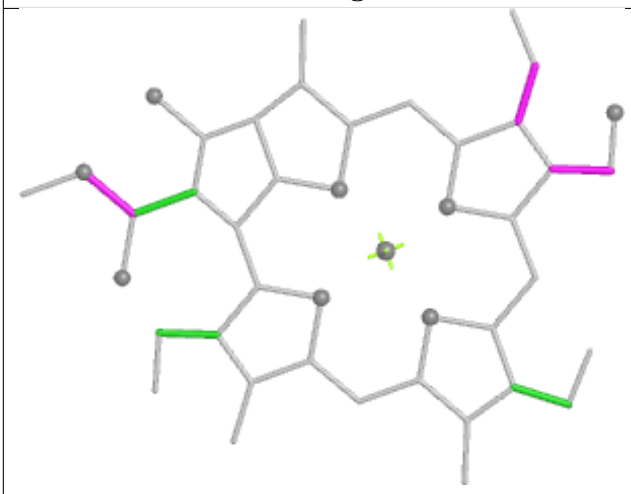
Ligand CHL 3 312



Bond lengths



Bond angles

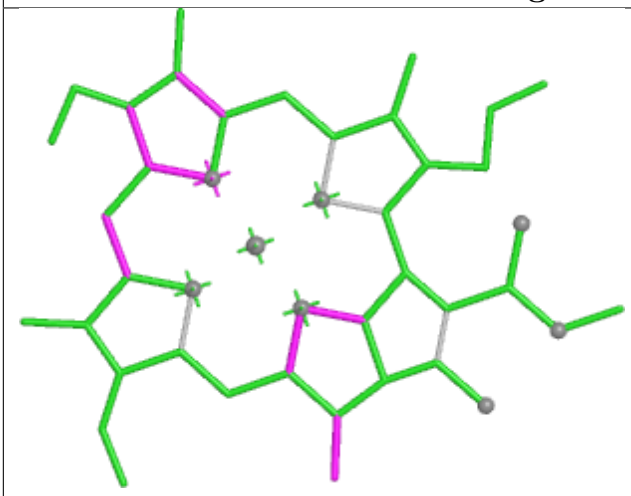


Torsions

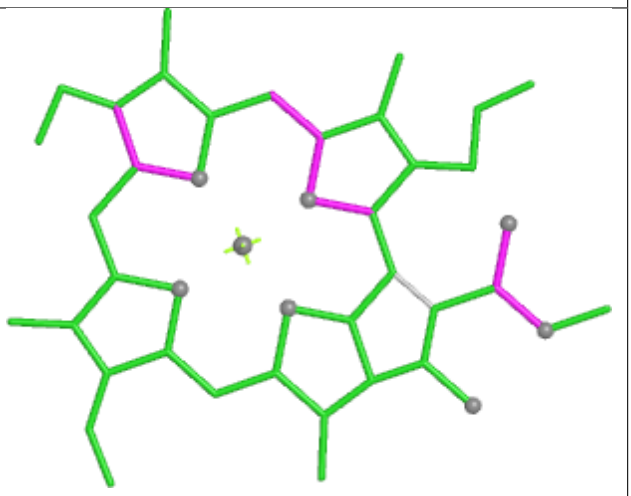


Rings

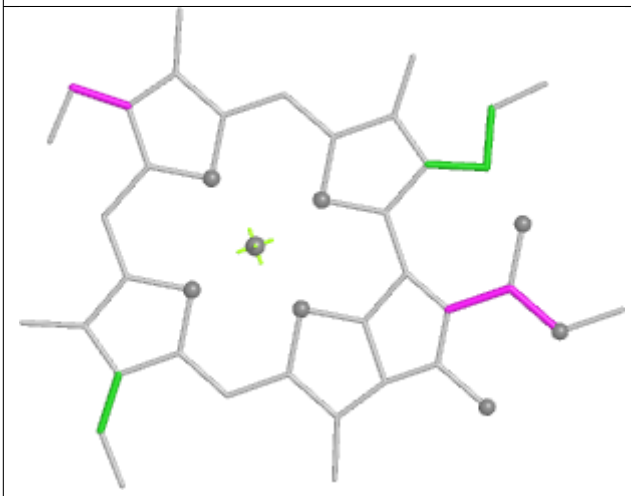
Ligand CLA 6 307



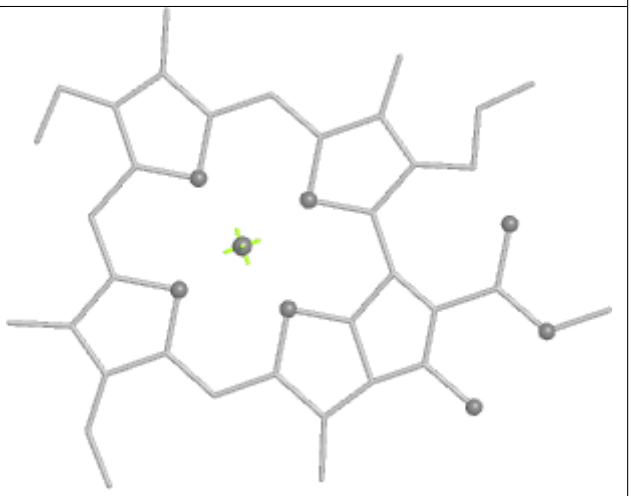
Bond lengths



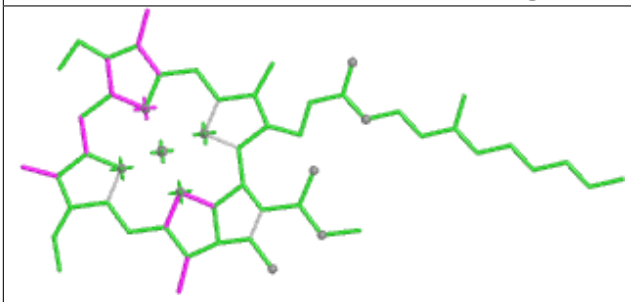
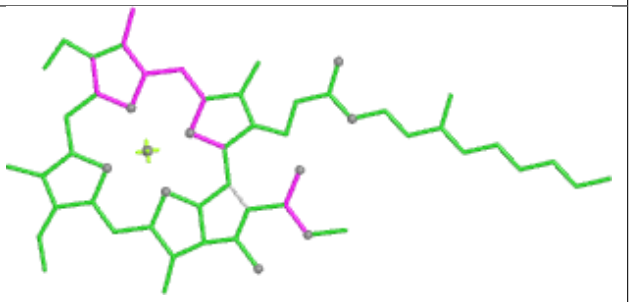
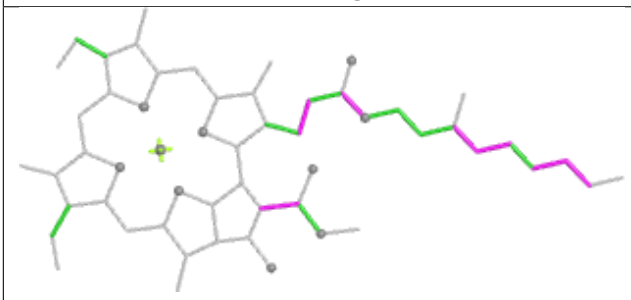
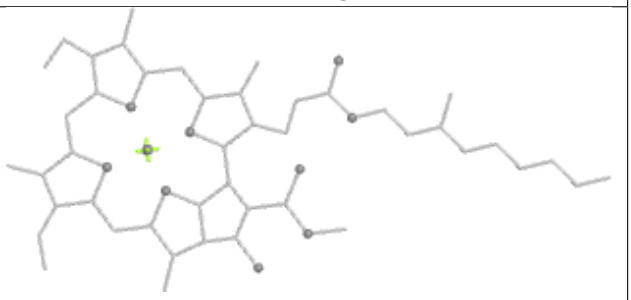
Bond angles



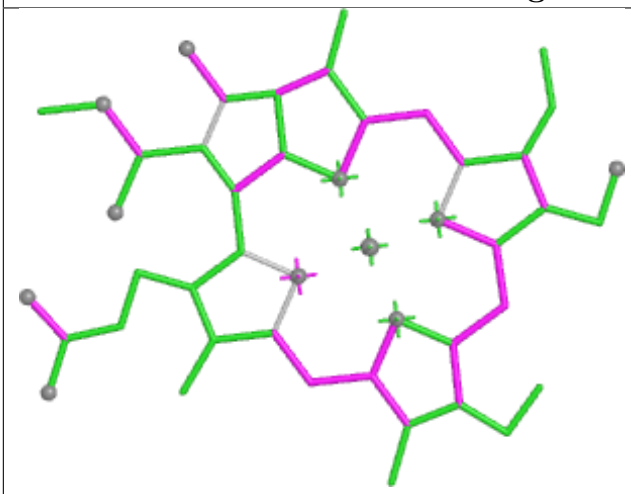
Torsions



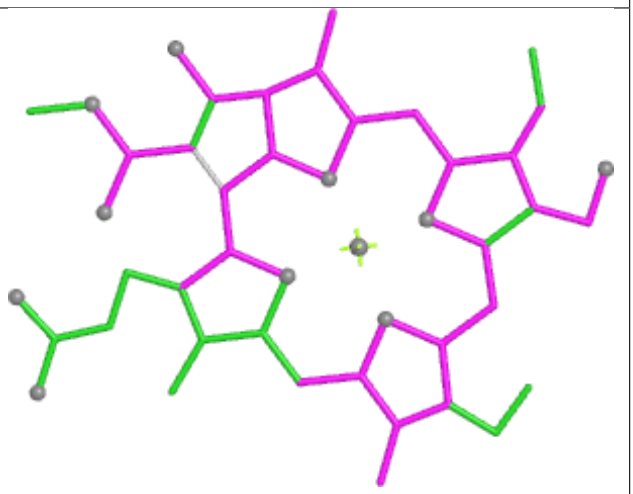
Rings

Ligand CLA Y 316	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

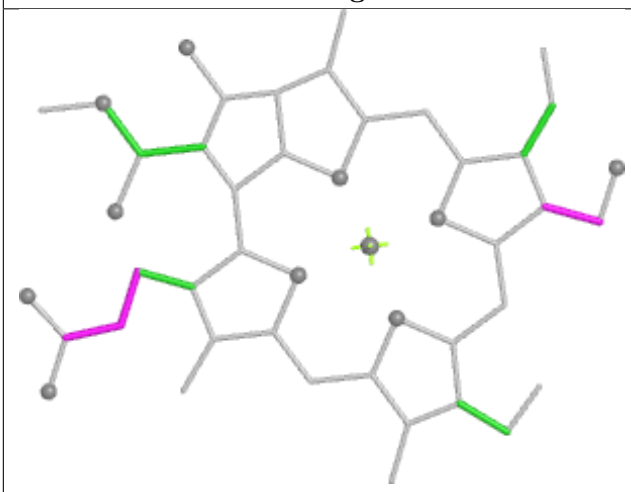
Ligand CHL 8 308



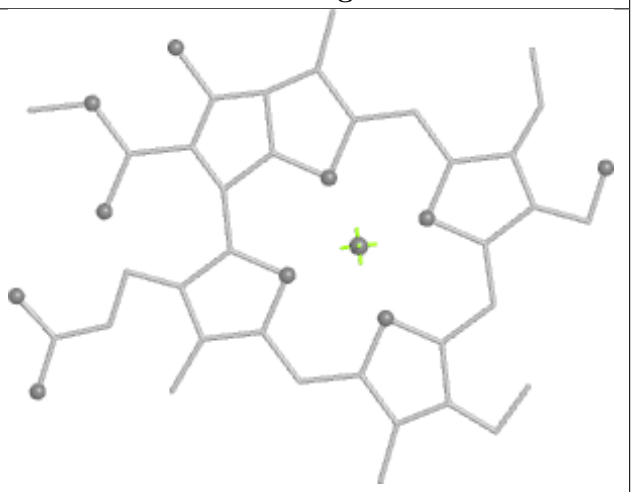
Bond lengths



Bond angles

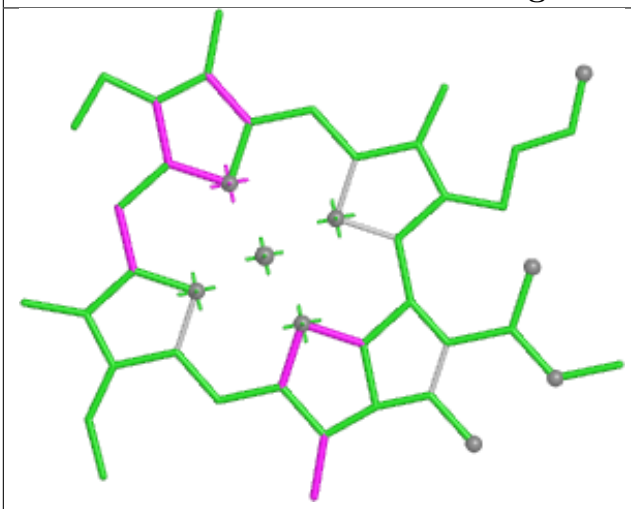


Torsions

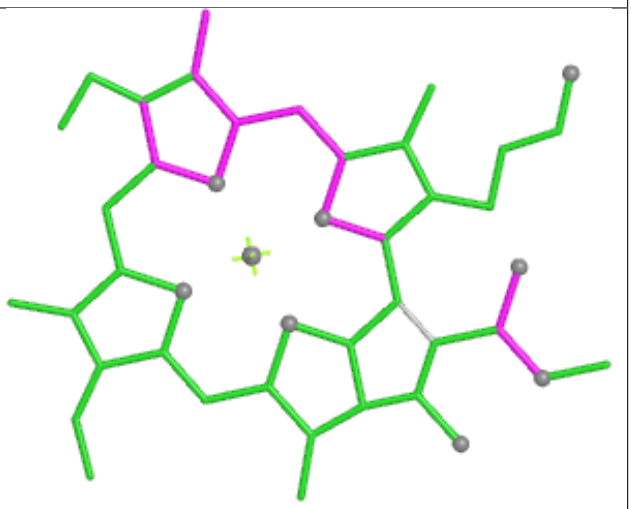


Rings

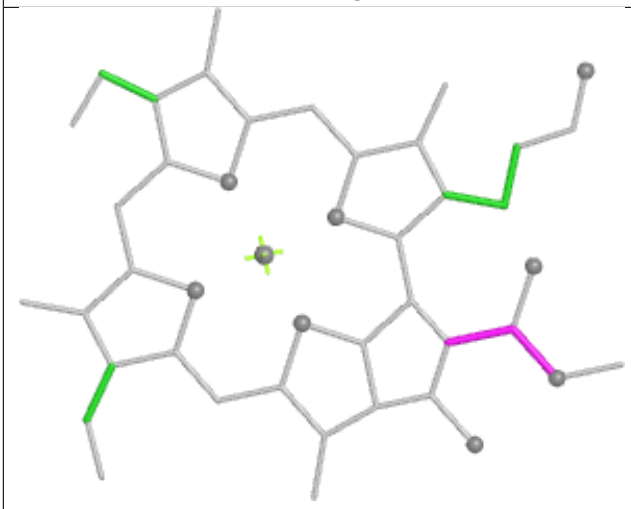
Ligand CLA 1 306



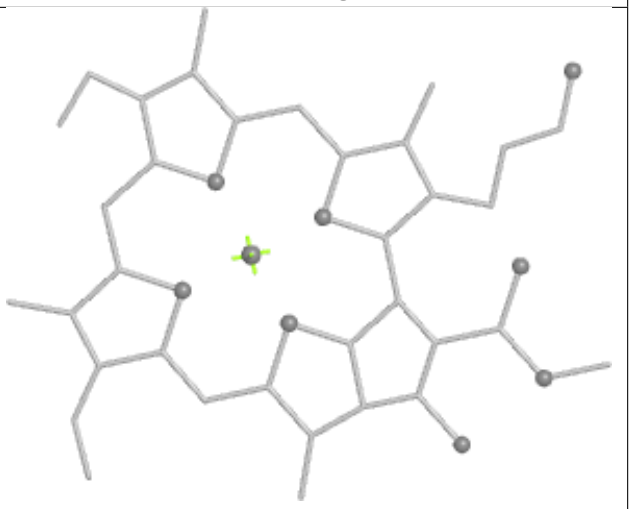
Bond lengths



Bond angles

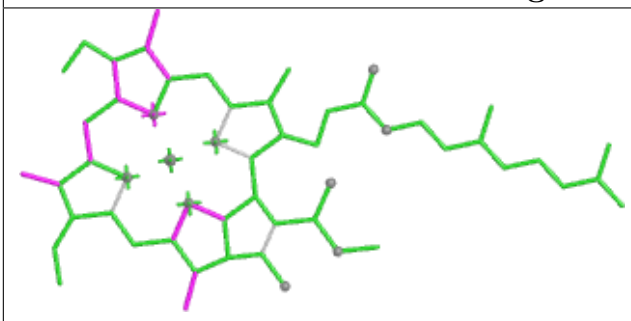


Torsions

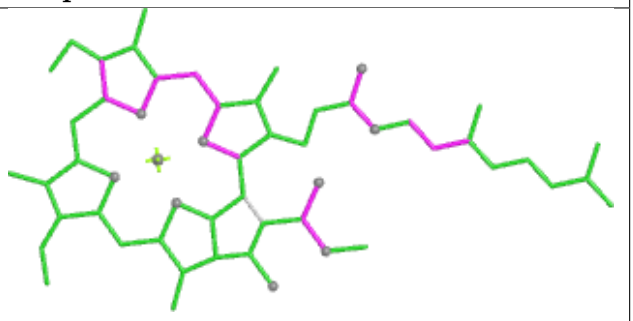


Rings

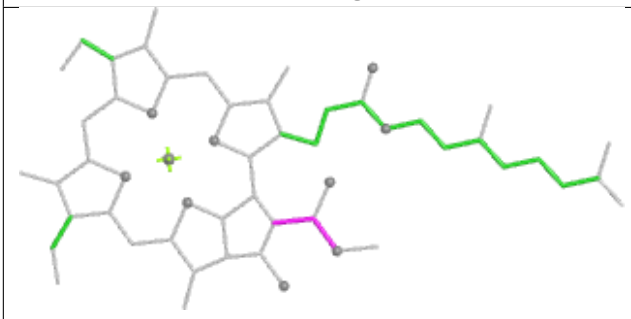
Ligand CLA q 312



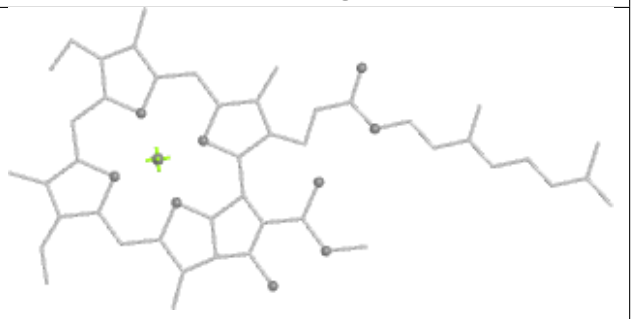
Bond lengths



Bond angles

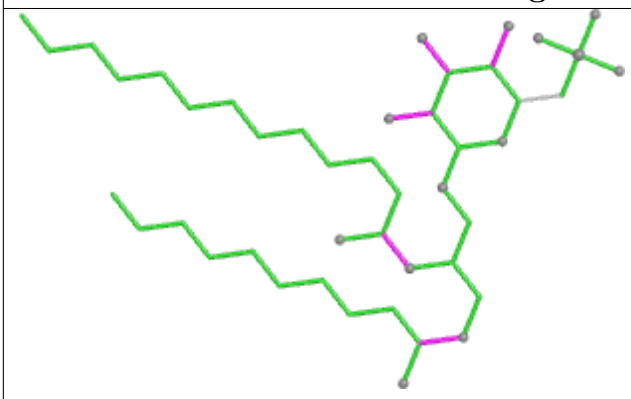


Torsions

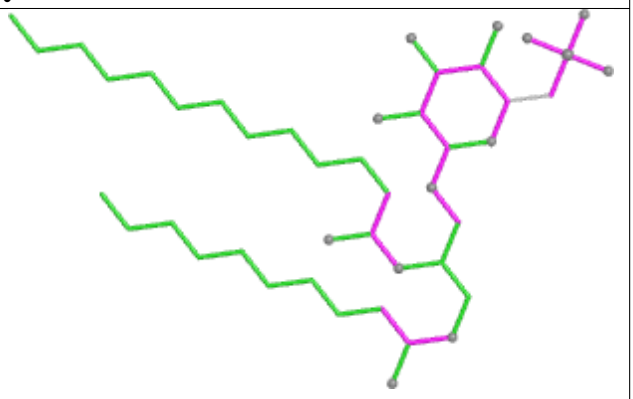


Rings

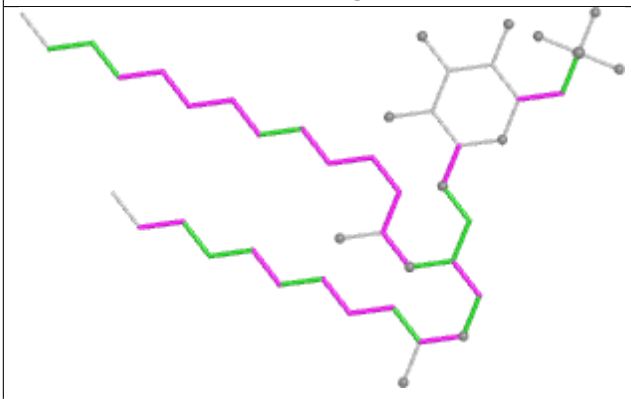
Ligand SQD a 609



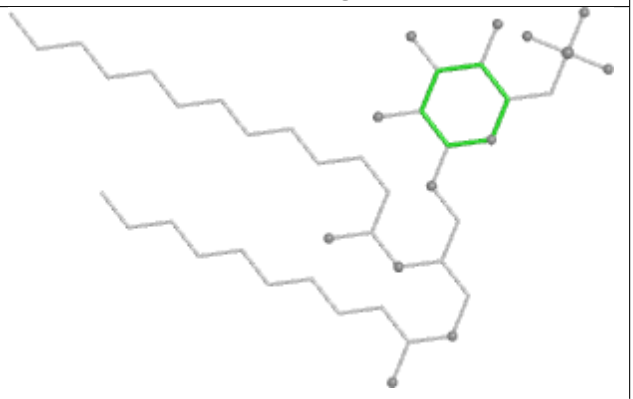
Bond lengths



Bond angles

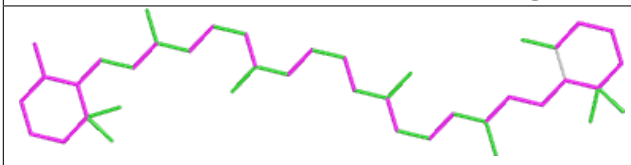


Torsions

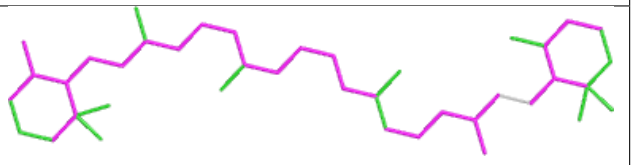


Rings

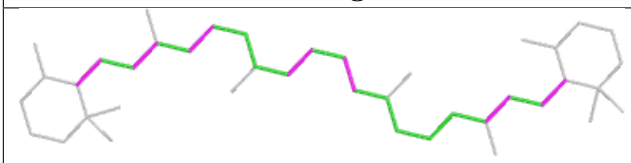
Ligand 8CT D 410



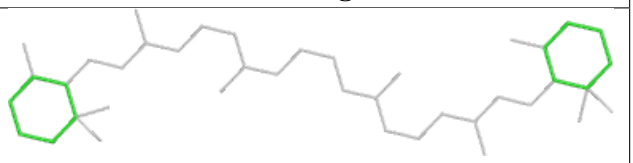
Bond lengths



Bond angles

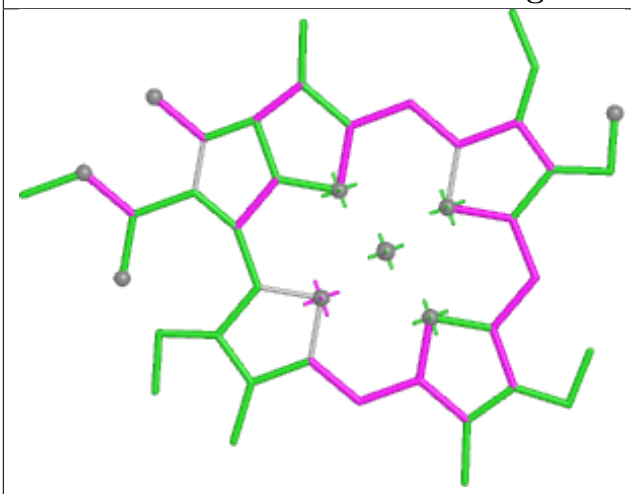


Torsions

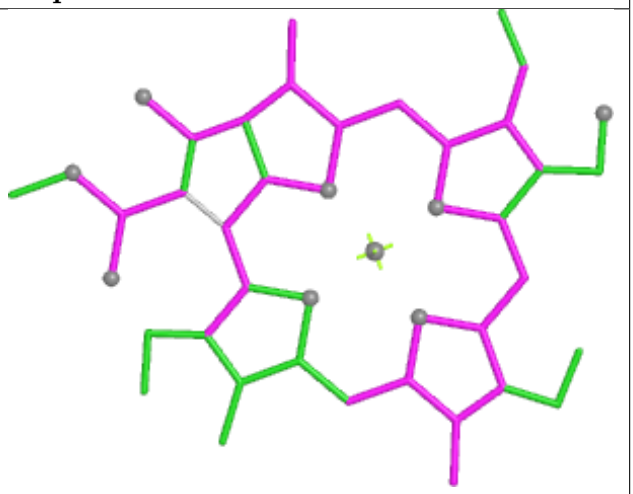


Rings

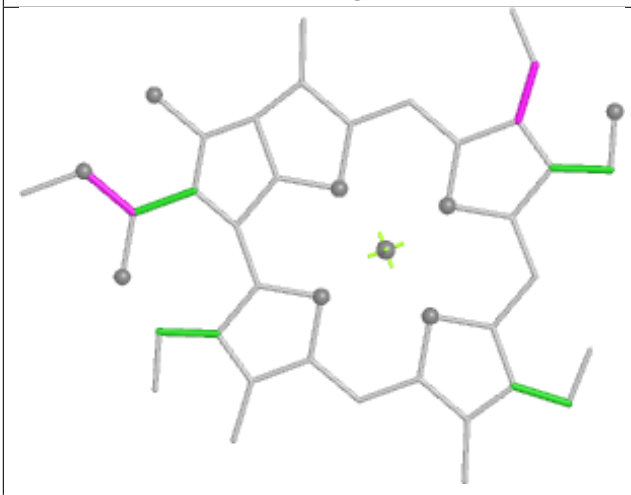
Ligand CHL p 313



Bond lengths



Bond angles

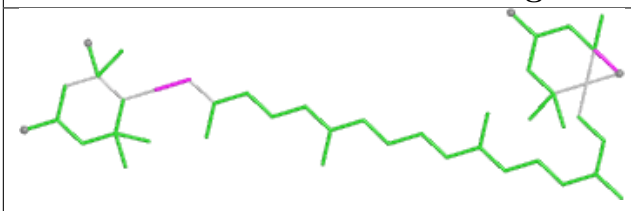


Torsions

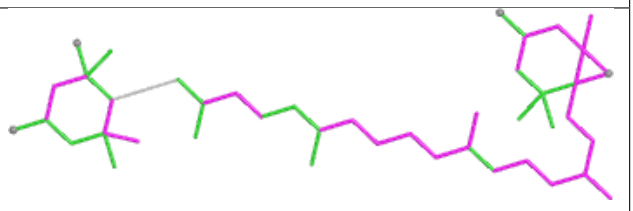


Rings

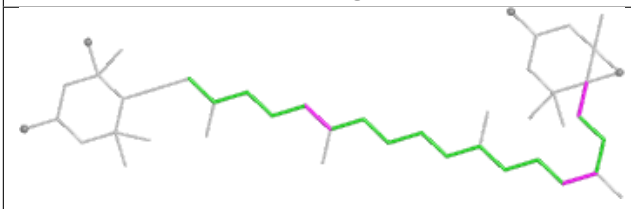
Ligand NEX n 303



Bond lengths



Bond angles

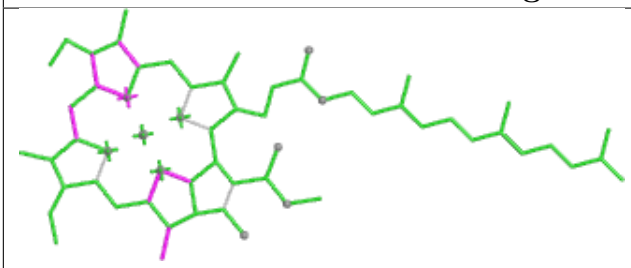


Torsions

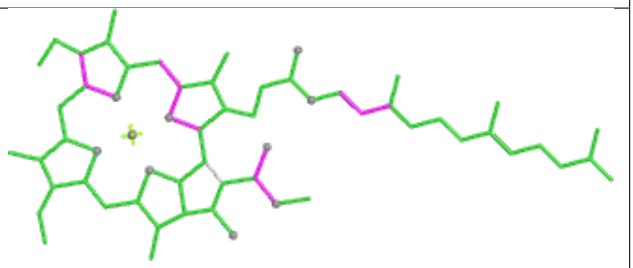


Rings

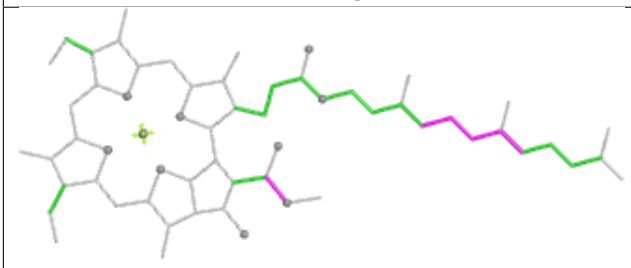
Ligand CLA G 315



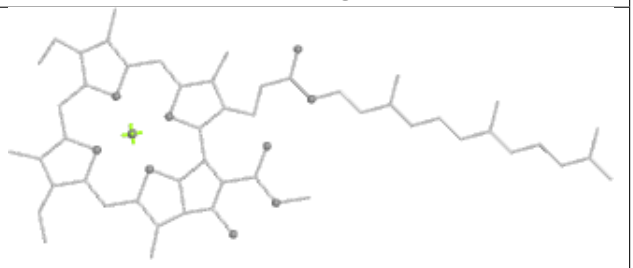
Bond lengths



Bond angles

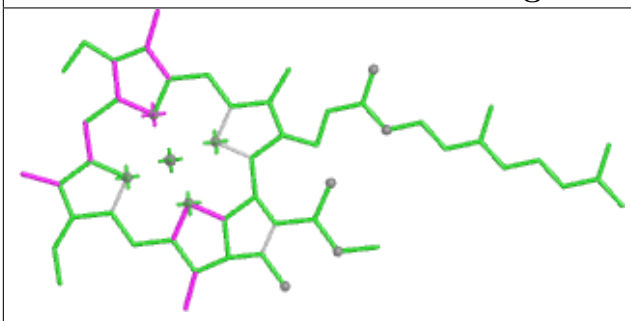


Torsions

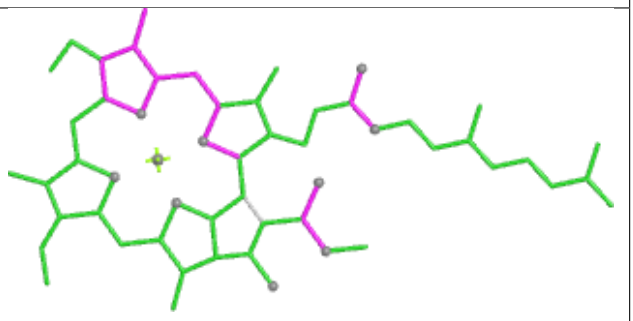


Rings

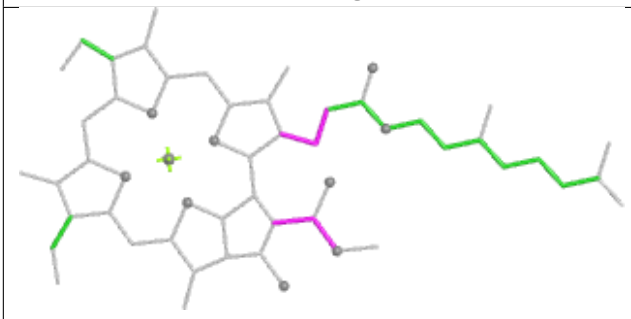
Ligand CLA Y 313



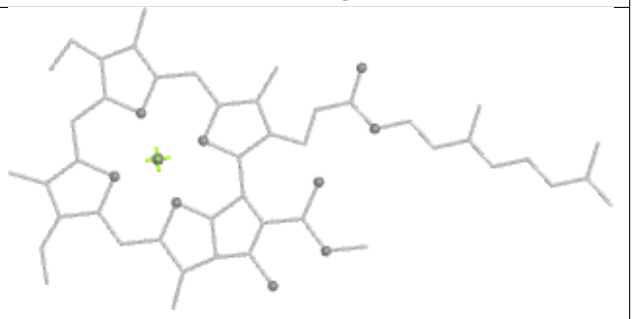
Bond lengths



Bond angles

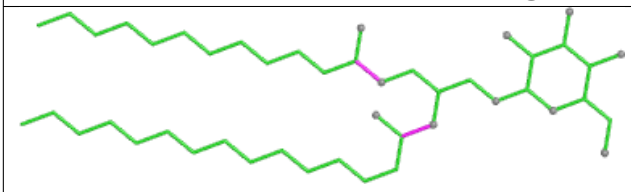


Torsions

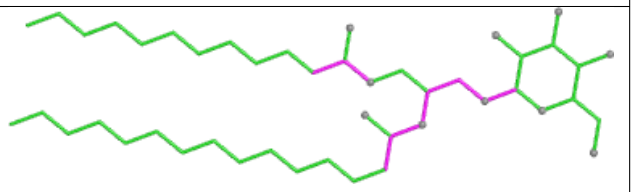


Rings

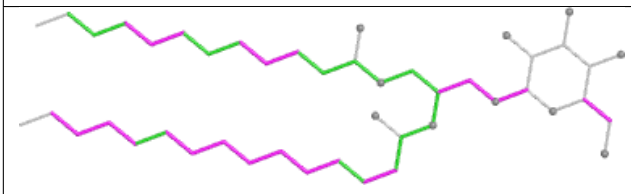
Ligand LMG d 411



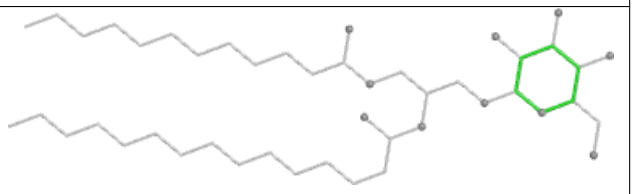
Bond lengths



Bond angles

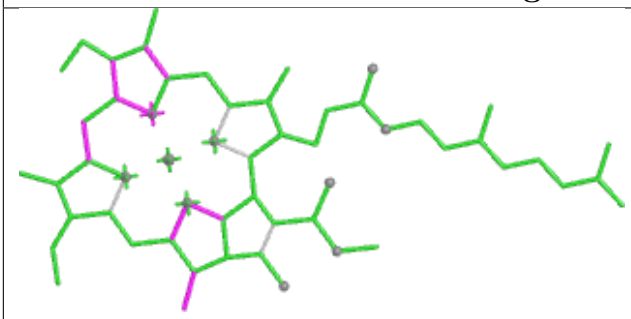


Torsions

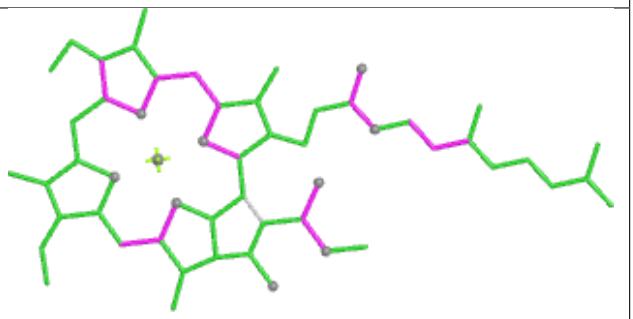


Rings

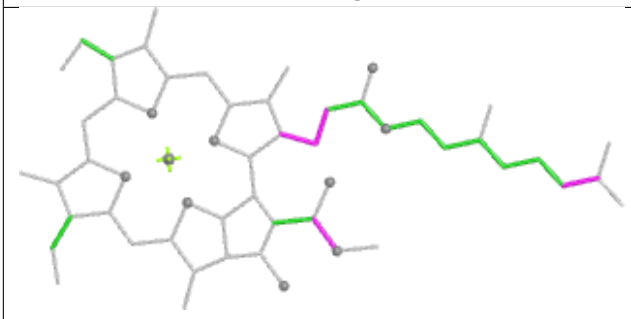
Ligand CLA N 313



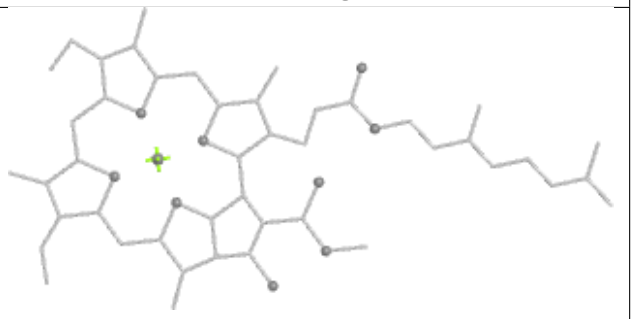
Bond lengths



Bond angles

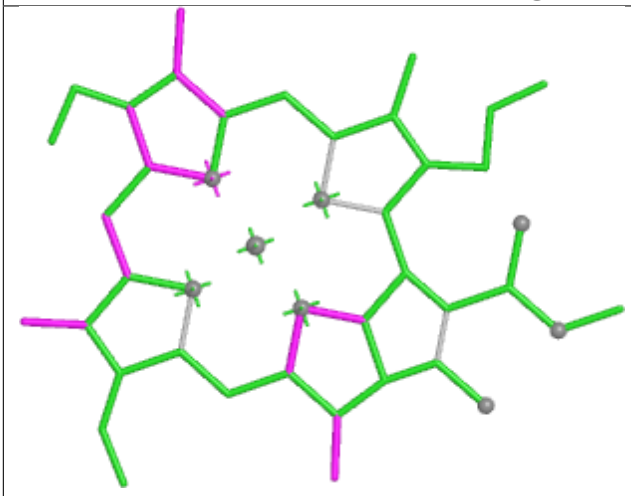


Torsions

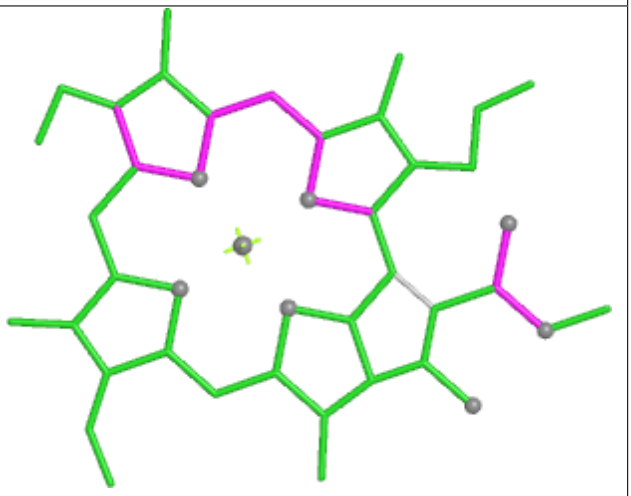


Rings

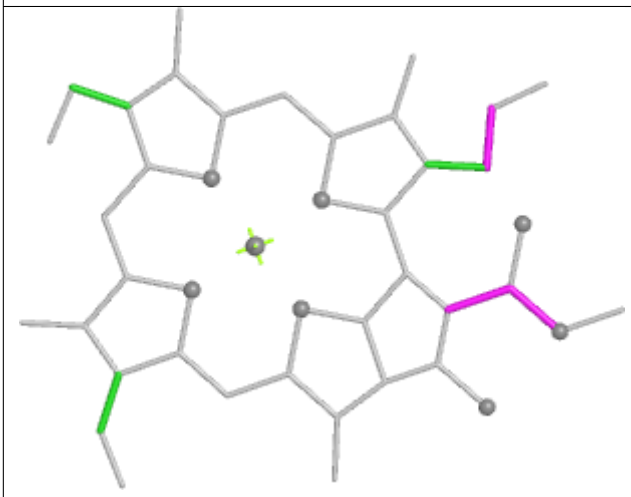
Ligand CLA 8 314



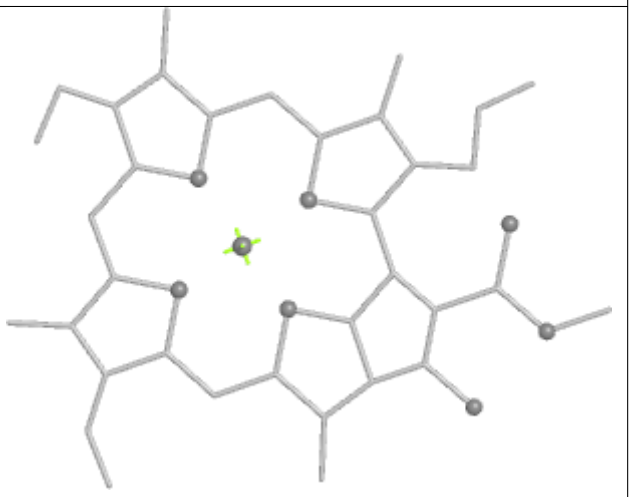
Bond lengths



Bond angles

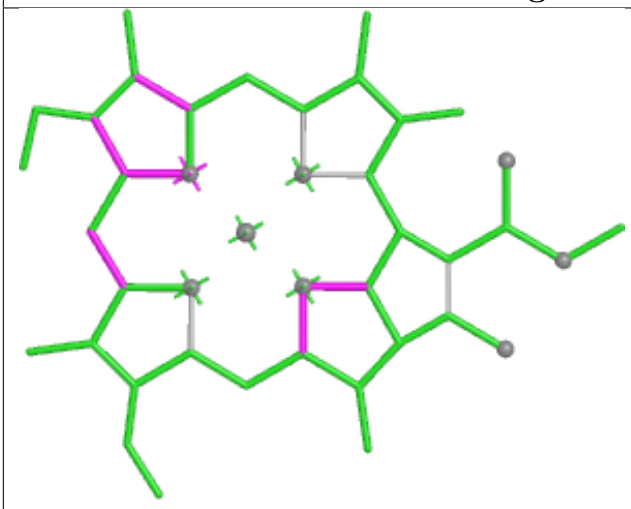


Torsions

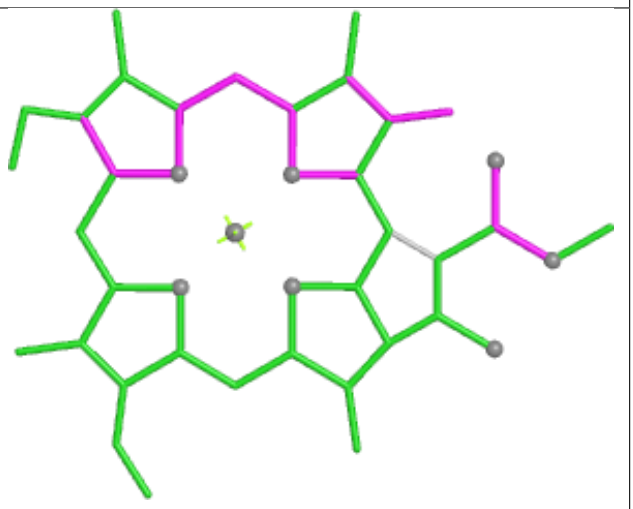


Rings

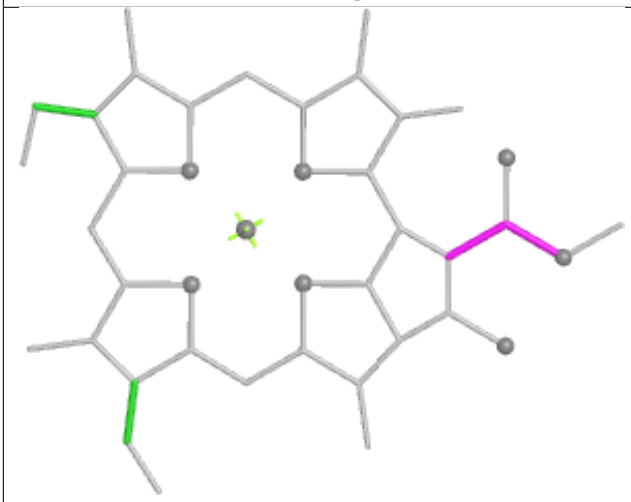
Ligand CLA 6 314



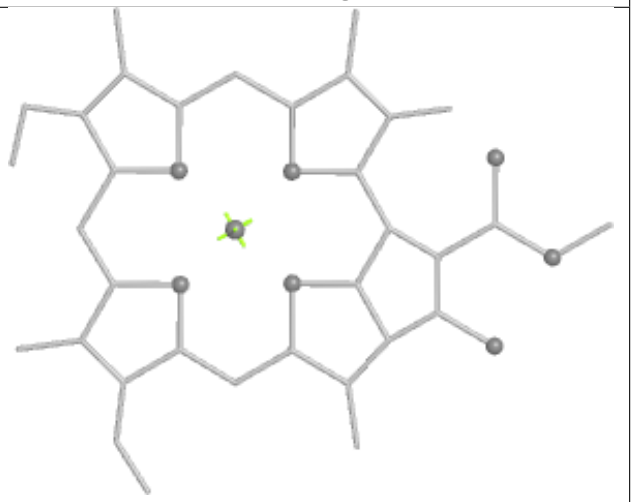
Bond lengths



Bond angles

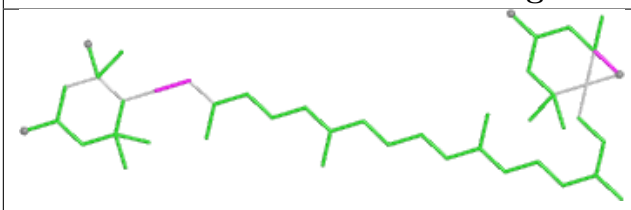


Torsions

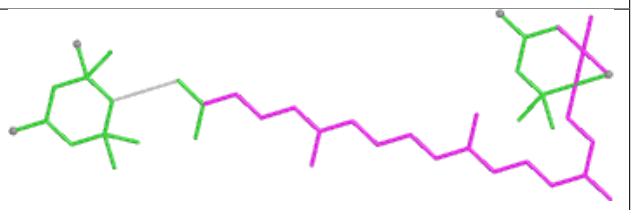


Rings

Ligand NEX 4 303



Bond lengths



Bond angles

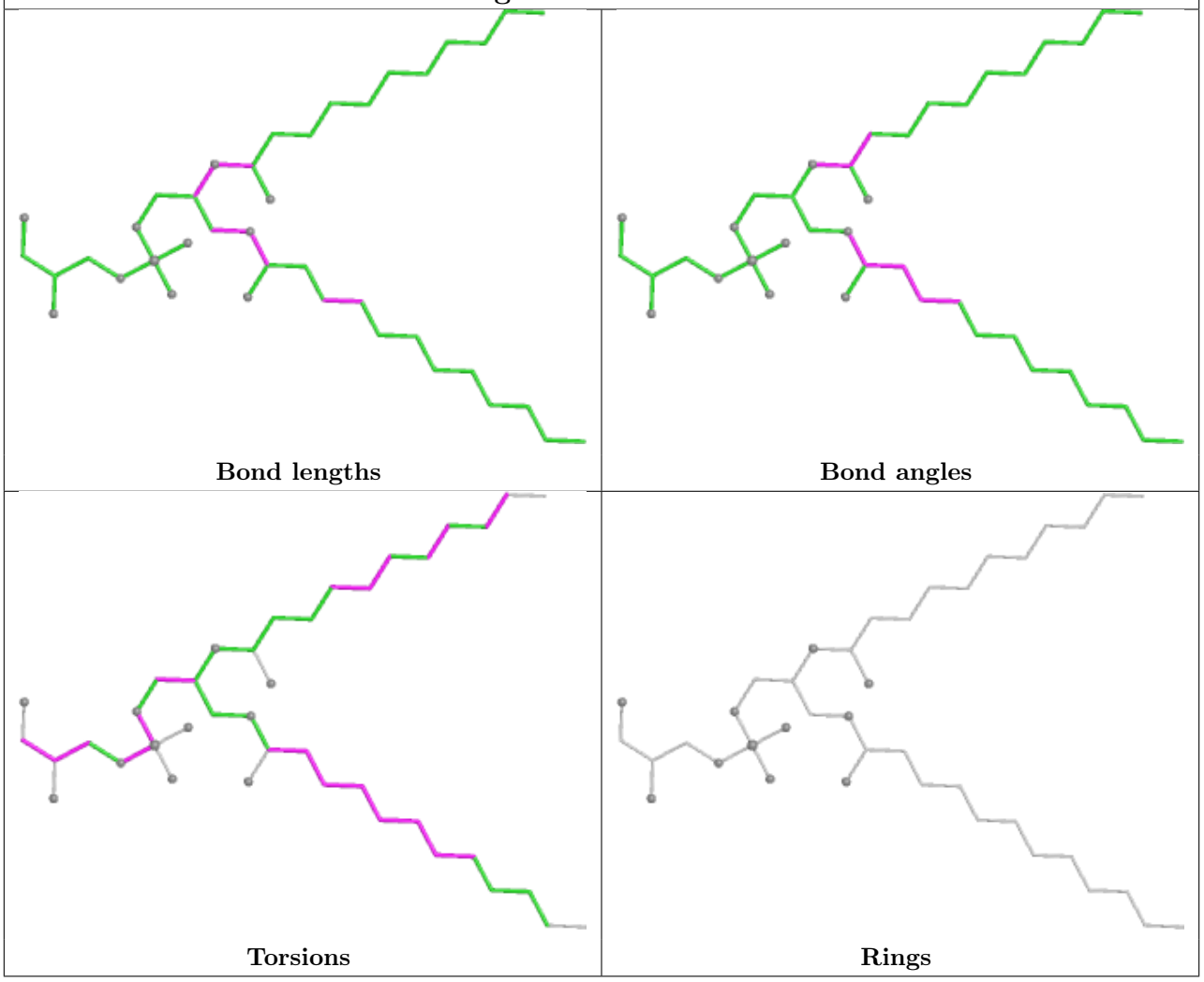


Torsions



Rings

Ligand LHG 2 319



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

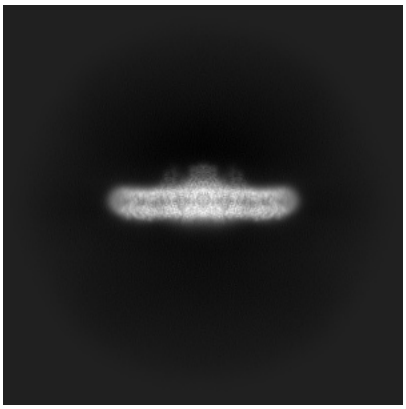
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62153. These allow visual inspection of the internal detail of the map and identification of artifacts.

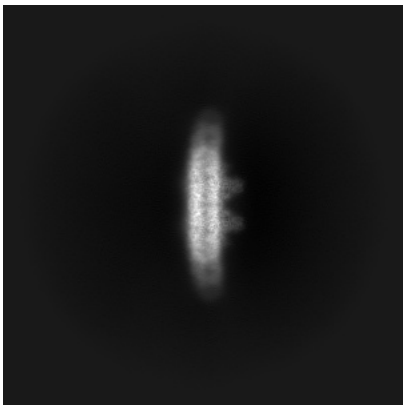
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

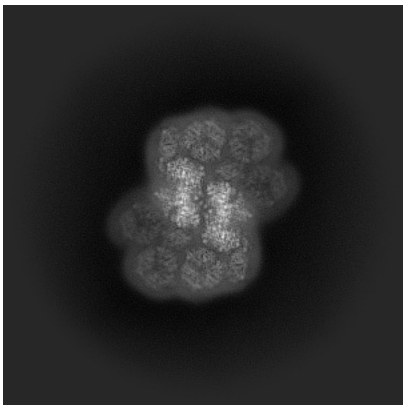
6.1.1 Primary map



X

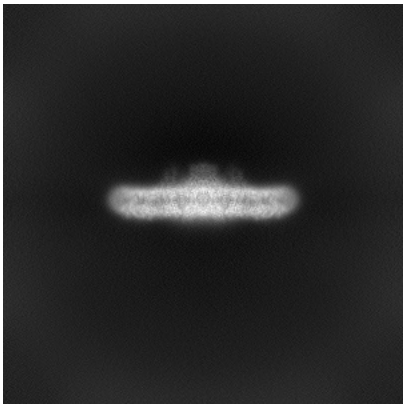


Y

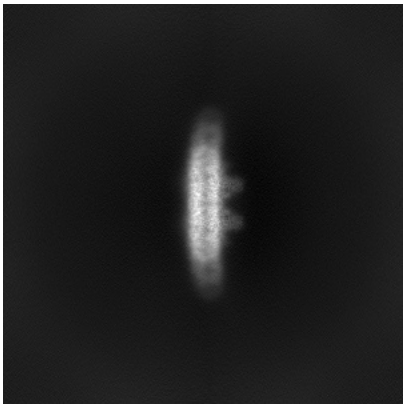


Z

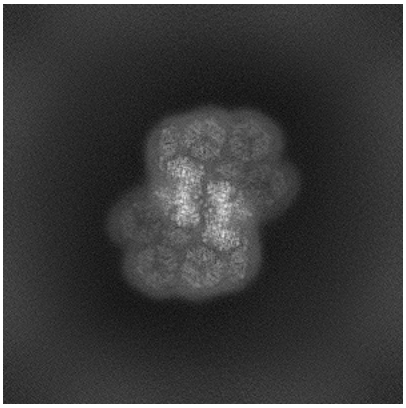
6.1.2 Raw map



X



Y

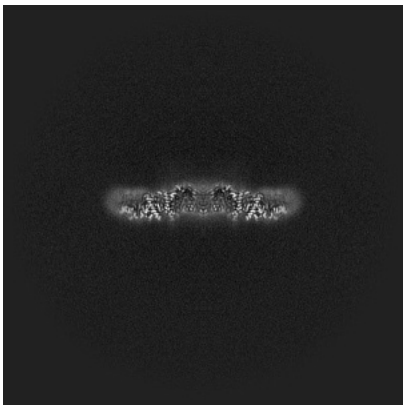


Z

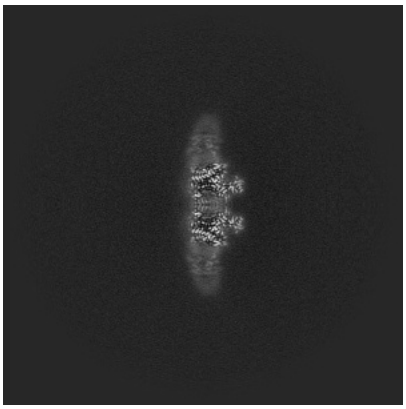
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

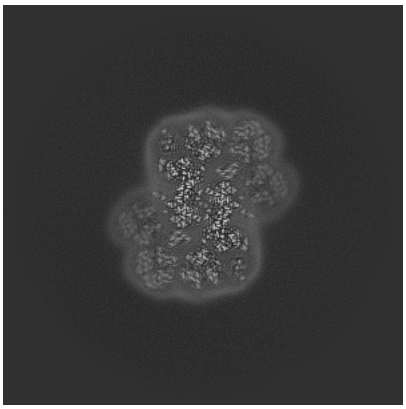
6.2.1 Primary map



X Index: 300

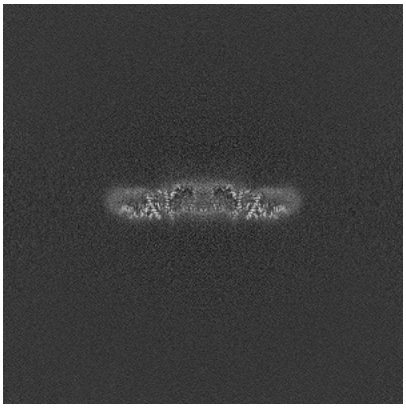


Y Index: 300

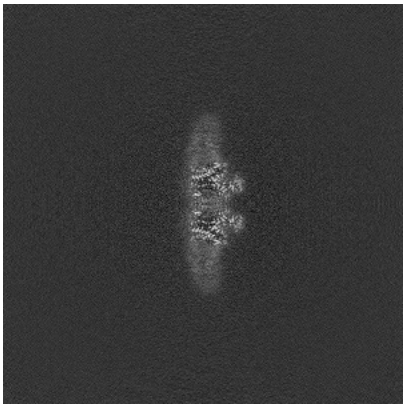


Z Index: 300

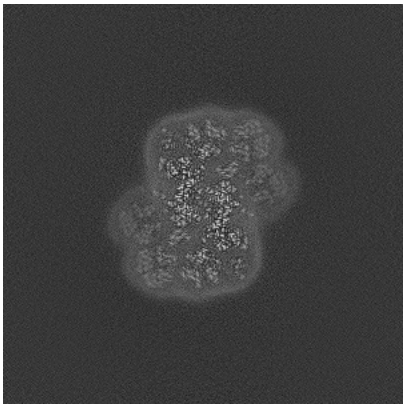
6.2.2 Raw map



X Index: 300



Y Index: 300

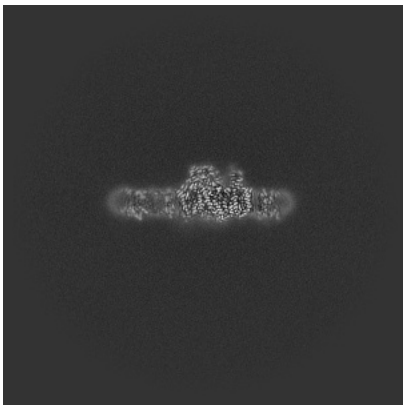


Z Index: 300

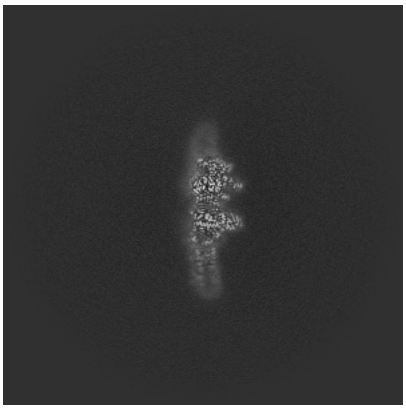
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

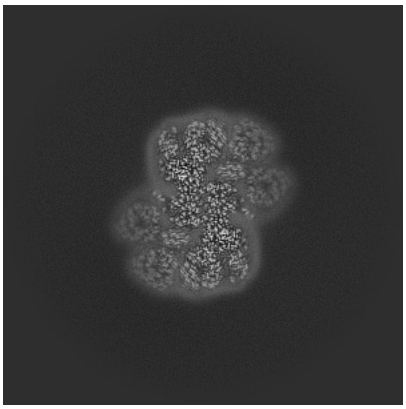
6.3.1 Primary map



X Index: 273

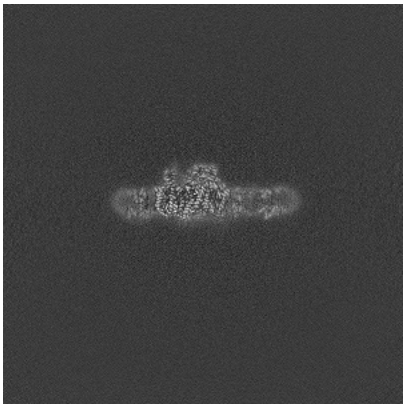


Y Index: 288

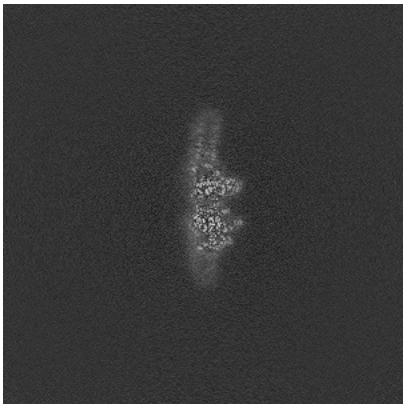


Z Index: 293

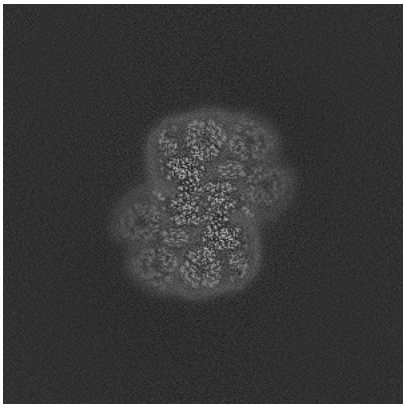
6.3.2 Raw map



X Index: 327



Y Index: 312

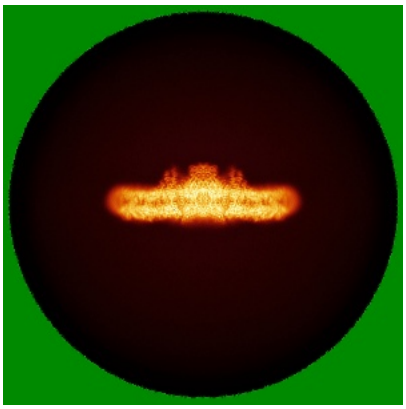


Z Index: 294

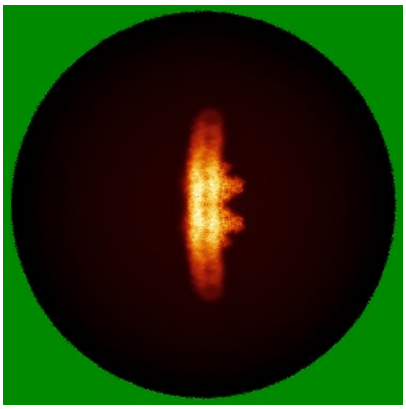
The images above show the largest variance slices of the map in three orthogonal directions.

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

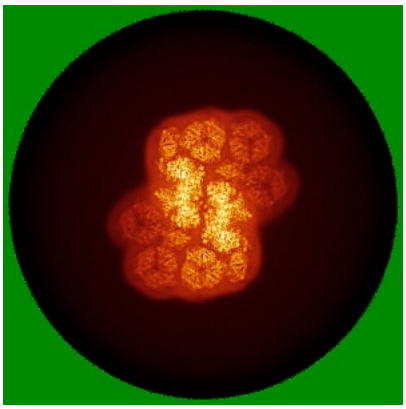
6.4.1 Primary map



X

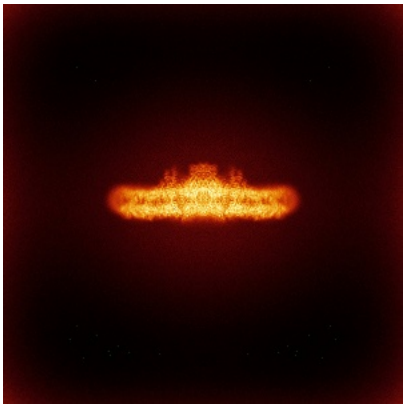


Y

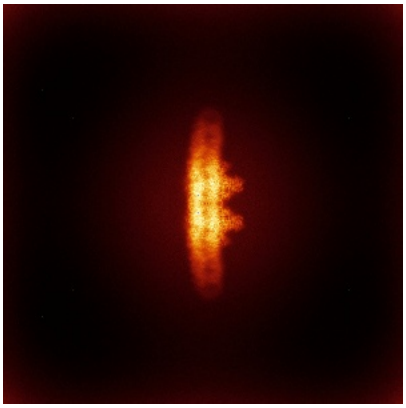


Z

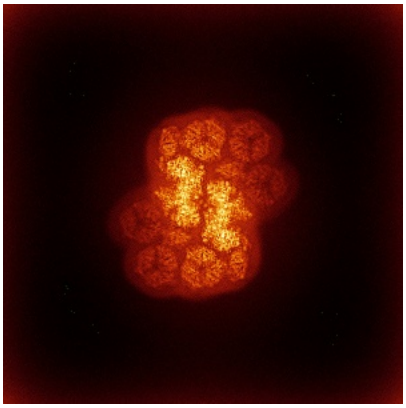
6.4.2 Raw map



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 0.204. 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.

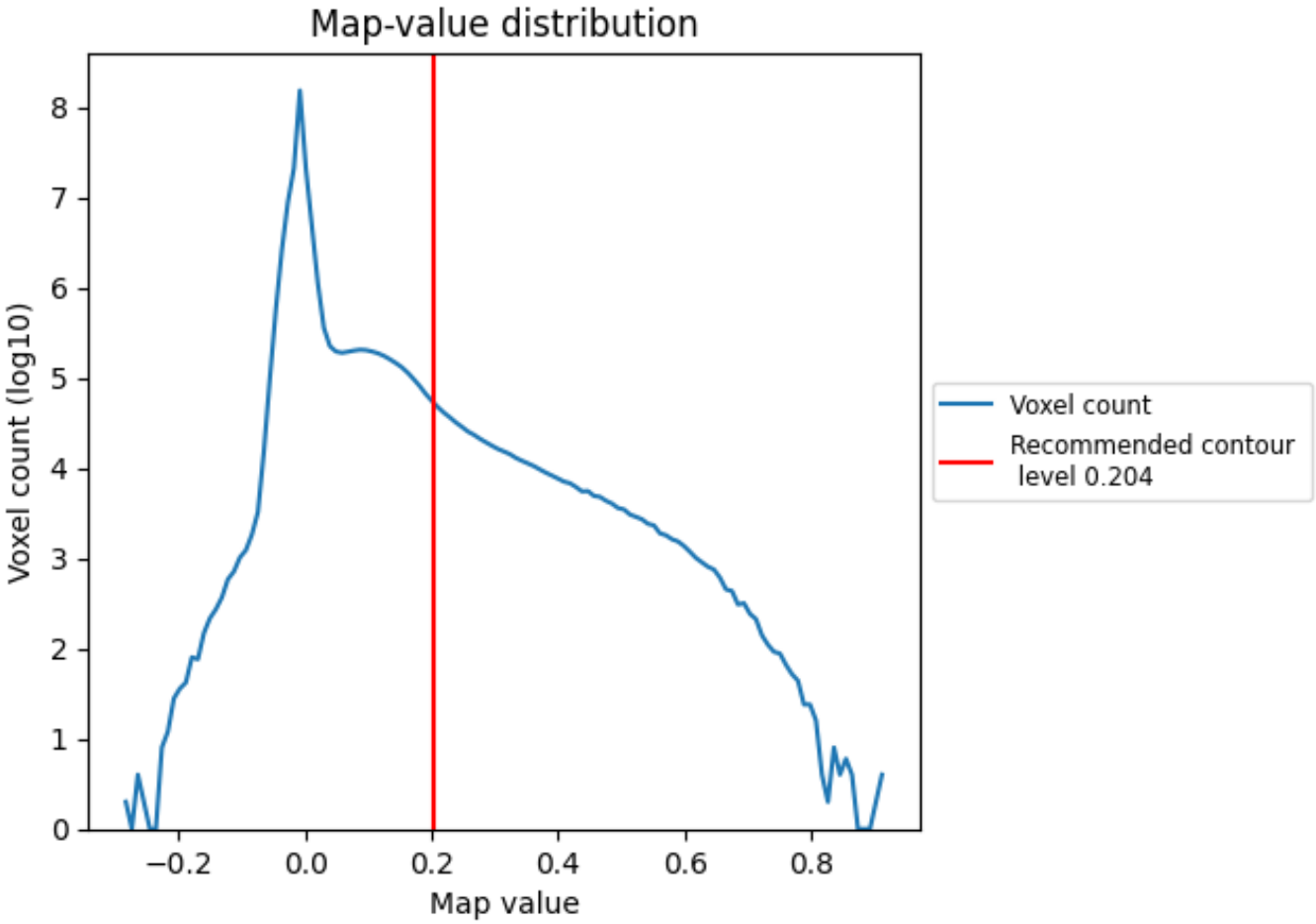
6.6 Mask visualisation (i)

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

7 Map analysis

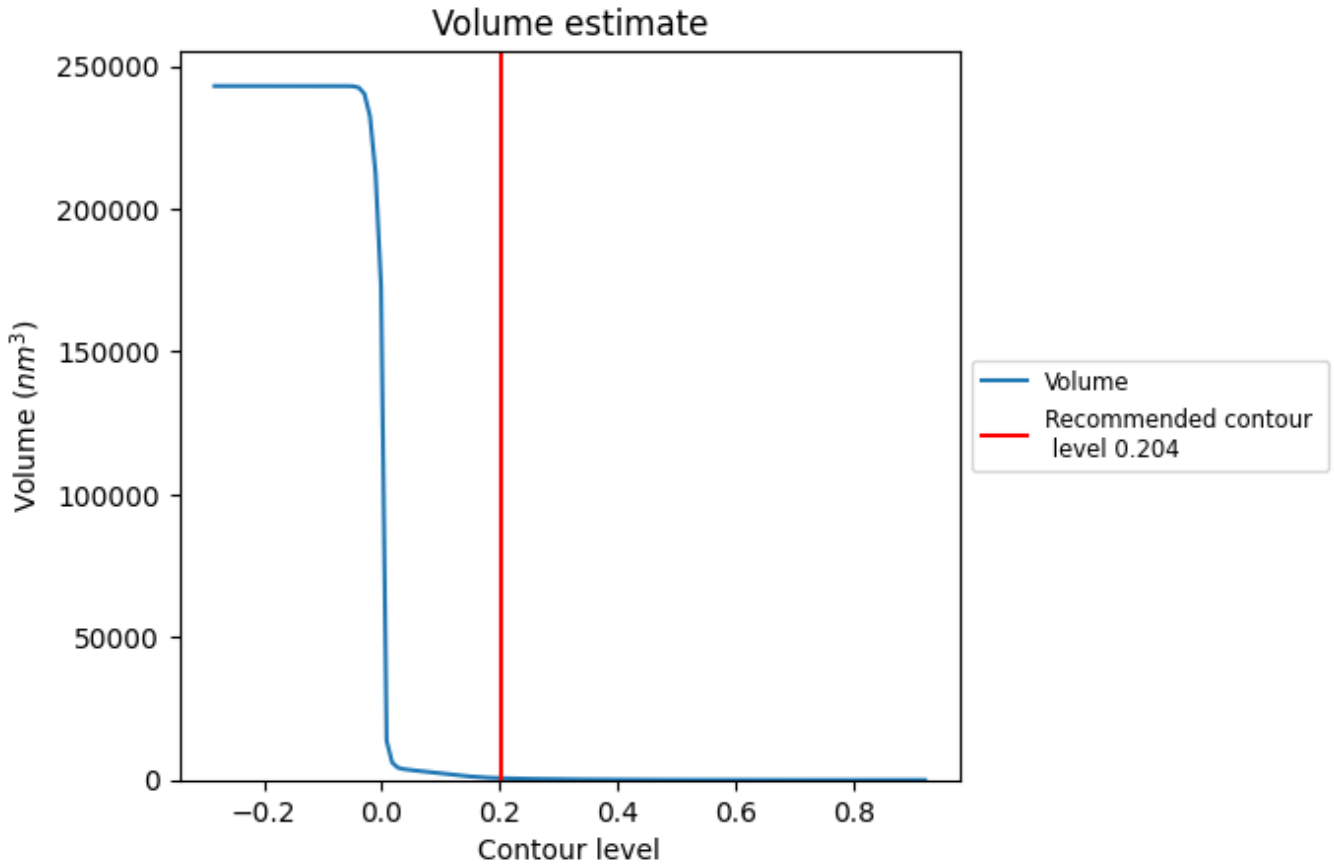
This section contains the results of statistical analysis of the map.

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.

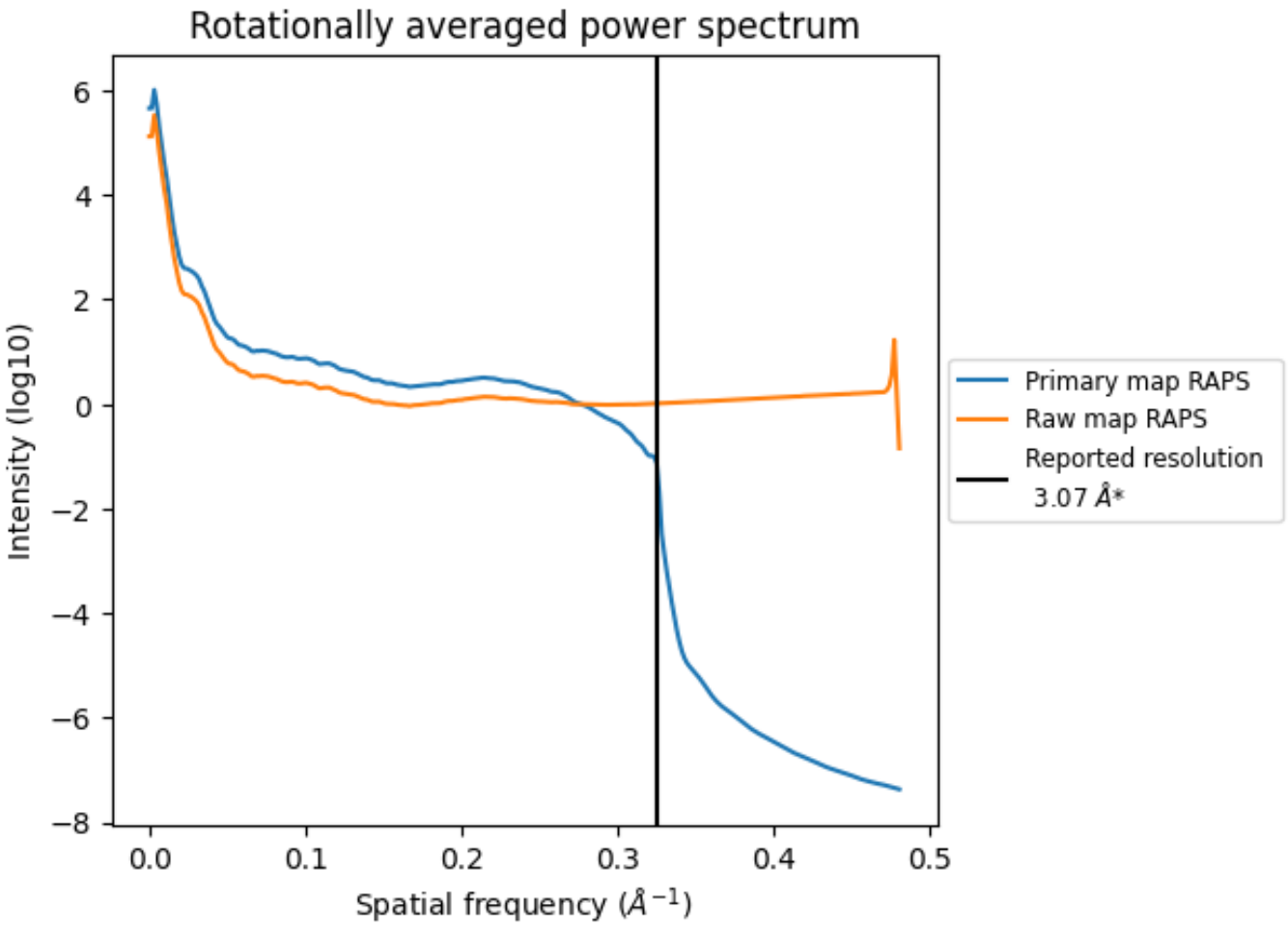
7.2 Volume estimate



The volume at the recommended contour level is 606 nm^3; this corresponds to an approximate mass of 548 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)

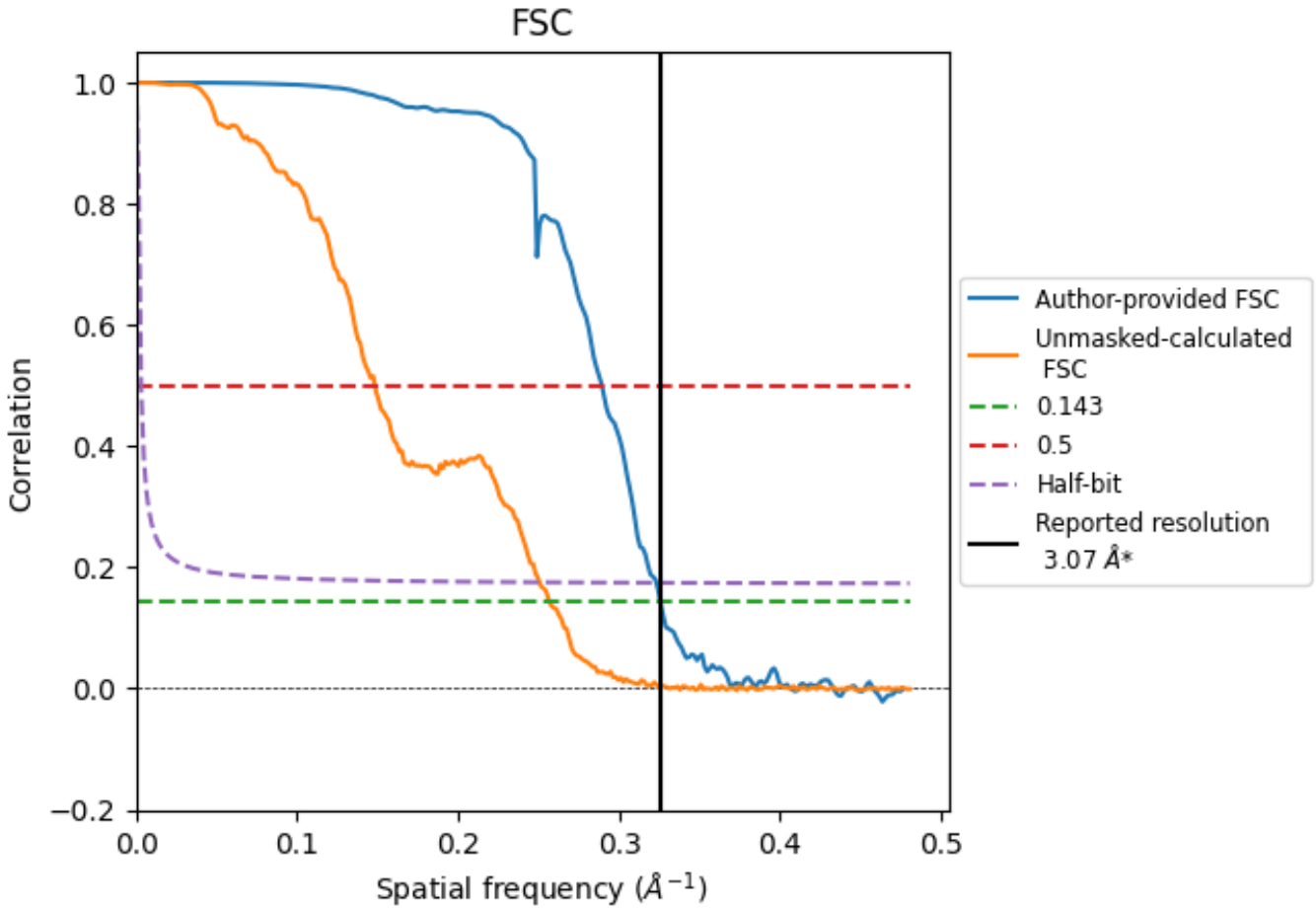


*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

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 0.326 Å^{-1}

8.2 Resolution estimates (i)

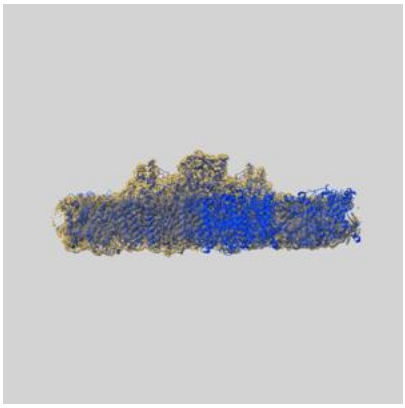
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.45	3.09
Unmasked-calculated*	3.89	6.74	3.99

*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 3.89 differs from the reported value 3.07 by more than 10 %

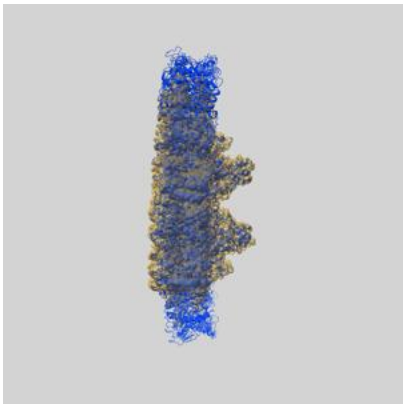
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62153 and PDB model 9K7V. Per-residue inclusion information can be found in section 3 on page 45.

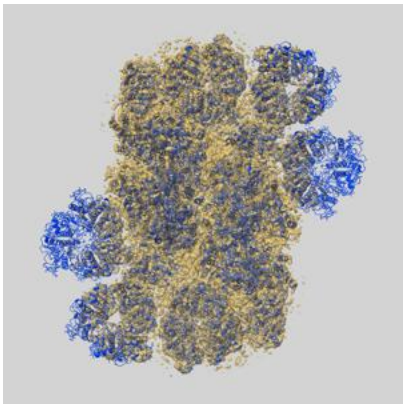
9.1 Map-model overlay



X



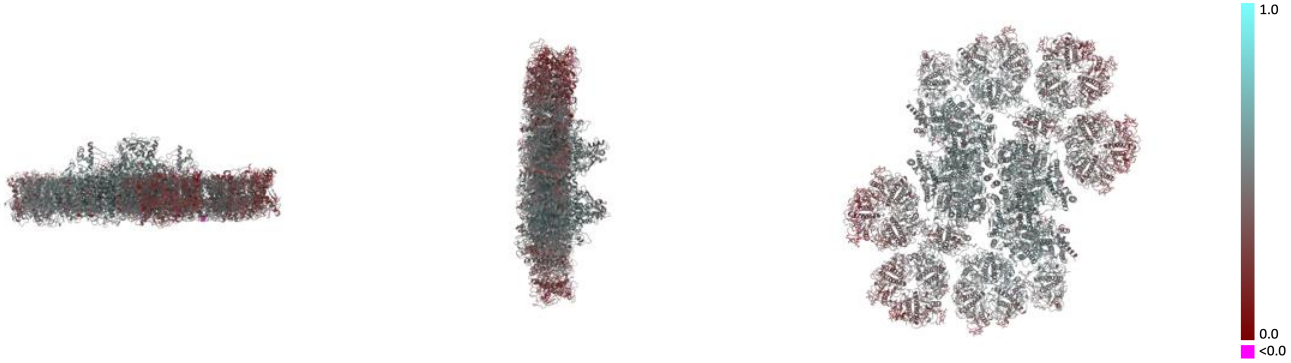
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.204 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.

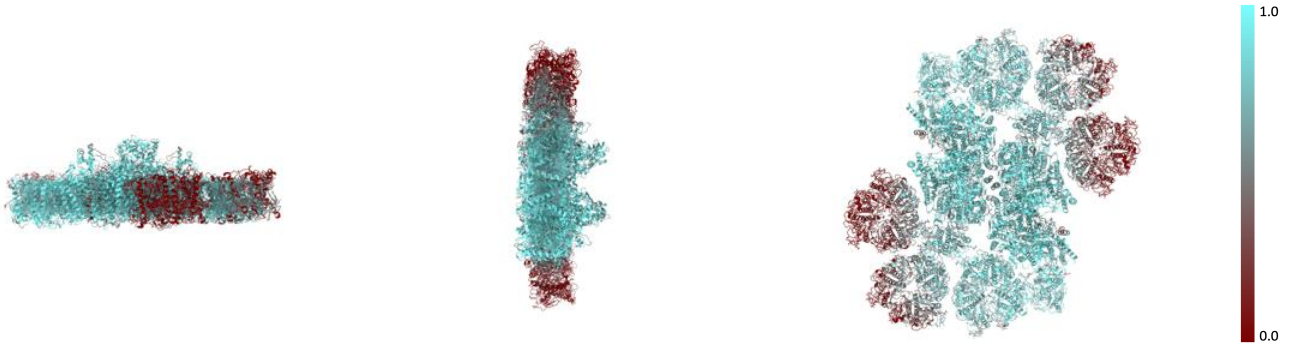
9.2 Q-score mapped to coordinate model (i)



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.

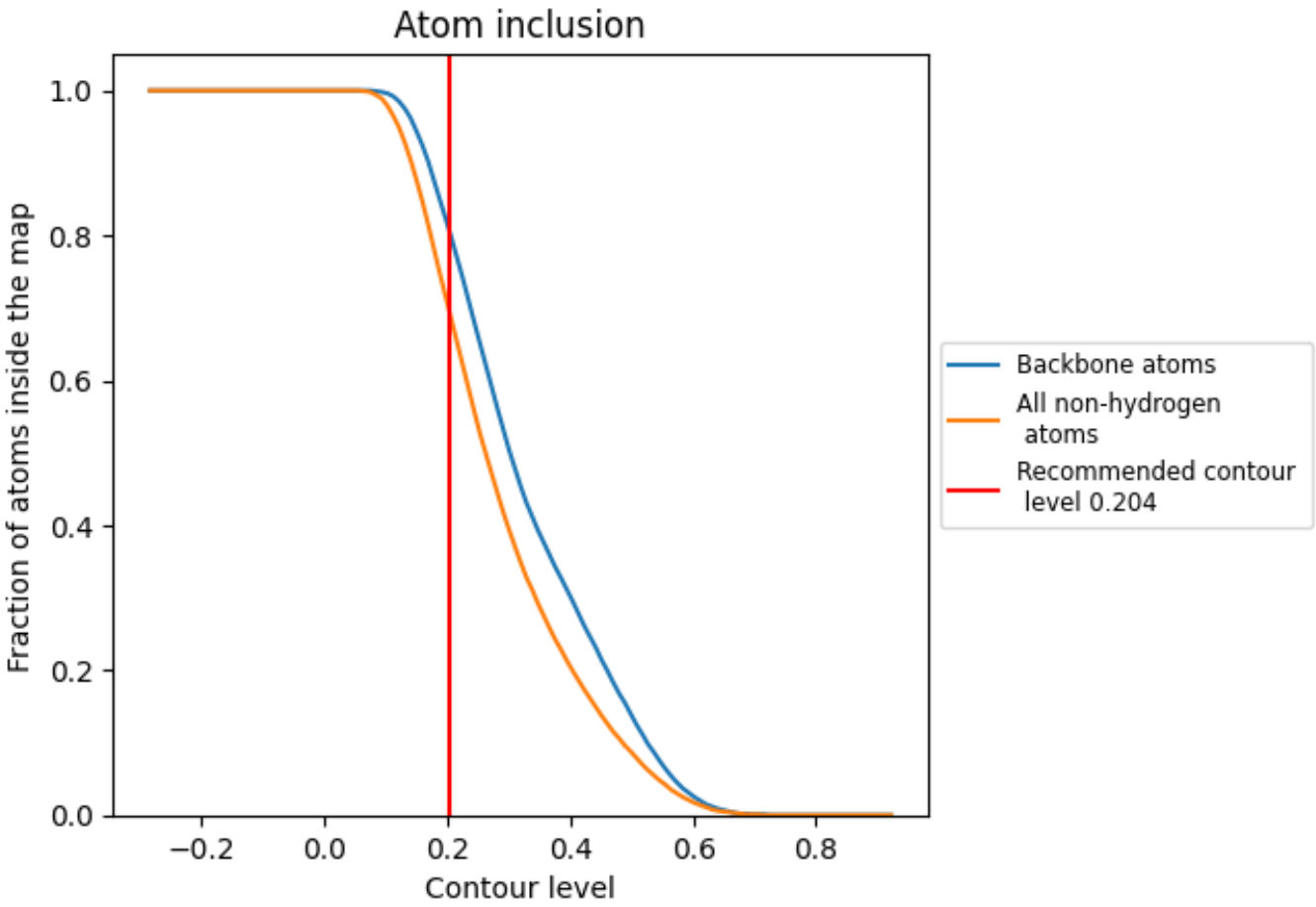
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.204).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.4550
1	0.3620	0.3400
2	0.6680	0.4570
3	0.3050	0.3320
4	0.3660	0.3380
5	0.6660	0.4580
6	0.3020	0.3250
7	0.7880	0.4340
8	0.8580	0.4730
9	0.0130	0.2470
A	0.9160	0.5370
B	0.9140	0.5310
C	0.9100	0.5370
D	0.9260	0.5490
E	0.8090	0.4670
F	0.8670	0.4710
G	0.2460	0.3830
H	0.8510	0.5070
I	0.9600	0.5430
K	0.9220	0.5170
L	0.9060	0.5290
M	0.7130	0.4500
N	0.3140	0.3920
R	0.7010	0.4140
S	0.8320	0.4570
T	0.8600	0.5220
V	0.4290	0.3920
W	0.9000	0.5010
X	0.8040	0.4860
Y	0.9010	0.5210
Z	0.8080	0.4380
a	0.9160	0.5370
b	0.9140	0.5320
c	0.9080	0.5350
d	0.9240	0.5490



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.8140	0.4640
f	0.8530	0.4640
g	0.2490	0.3850
h	0.8430	0.5070
i	0.9500	0.5570
k	0.9290	0.5150
l	0.9100	0.5340
m	0.7310	0.4650
n	0.3180	0.3910
p	0.7870	0.4340
q	0.8550	0.4720
r	0.7020	0.4130
s	0.8340	0.4560
t	0.8640	0.5190
u	0.0150	0.2460
v	0.4470	0.3850
w	0.8840	0.4930
x	0.7970	0.4900
y	0.8990	0.5210
z	0.8080	0.4370