Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 01:50 PM JST

PDB ID	:	9LE7 / pdb_00009le7
EMDB ID	:	EMD-63017
Title	:	Coordinates of Cryo-EM structure of the Arabidopsis thaliana C4S4M4-type PSII supercomplex
Authors	:	Chen, S.J.B.; Wu, C.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on	:	2025-01-07
Resolution	:	3.80 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 (i) symbol.

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

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

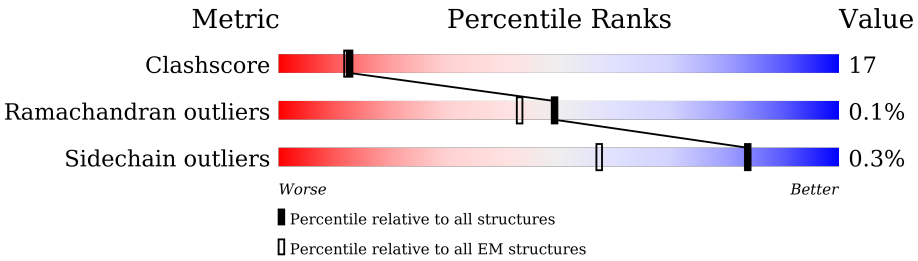
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

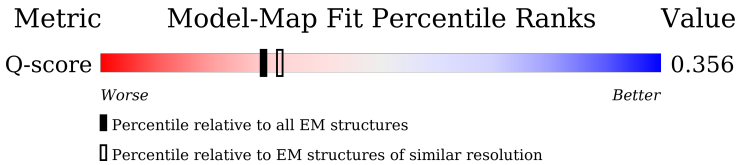
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	5	266	50% 25% 24%
1	7	266	49% 26% 24%
1	9	266	49% 27% 24%
1	AA	266	48% 27% 24%

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Mol	Chain	Length	Quality of chain
2	0	243	53% 37% 9%
2	6	243	53% 37% 9%
3	8	212	54% 36% 9%
3	AB	212	52% 38% 9%
4	B	508	76% 18% 6%
4	BE	508	78% 16% 6%
4	b	508	77% 17% 6%
4	v	508	77% 17% 6%
5	2	352	82% 15%
5	BG	352	75% 21%
5	D	352	81% 16%
5	d	352	72% 25%
6	3	83	58% 22% 20%
6	BH	83	49% 30% 20%
6	E	83	55% 24% 20%
6	e	83	53% 27% 20%
7	4	39	41% 33% 26%
7	BI	39	41% 33% 26%
7	F	39	41% 33% 26%
7	f	39	46% 28% 26%
8	A2	232	67% 20% 13%
8	Au	232	67% 22% 11%
8	BB	232	72% 19% 8%
8	BJ	232	68% 21% 11%
8	BQ	232	65% 22% 13%

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Mol	Chain	Length	Quality of chain
8	Ba	232	70% 21% 8%
8	G	232	67% 22% 11%
8	N	232	66% 21% 13%
8	Y	232	71% 20% 8%
8	g	232	69% 20% 11%
8	n	232	65% 22% 13%
8	y	232	69% 22% 8%
9	Av	72	53% 29% 18%
9	BK	72	56% 25% 18%
9	H	72	62% 18% 18%
9	h	72	49% 32% 18%
10	Aw	36	89% 8%
10	BL	36	6% 67% 31%
10	I	36	78% 19%
10	i	36	6% 58% 39%
11	Ay	37	89% 11%
11	BN	37	5% 84% 16%
11	K	37	89% 11%
11	k	37	5% 73% 27%
12	Az	38	5% 68% 24% 8%
12	BO	38	63% 29% 8%
12	L	38	5% 63% 29% 8%
12	l	38	61% 32% 8%
13	A1	34	50% 44% 6%
13	BP	34	56% 35% 6%

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Mol	Chain	Length	Quality of chain
13	M	34	56% 32% 6% 6%
13	m	34	50% 41% • 6%
14	A6	232	• 75% 18% 7%
14	BV	232	11% 62% 31% 7%
14	S	232	74% 19% 7%
14	s	232	12% 66% 27% 7%
15	A7	33	• 58% 27% • 12%
15	BW	33	6% 67% 21% 12%
15	T	33	• 55% 33% 12%
15	t	33	6% 55% 33% 12%
16	A8	28	25% 64% 25% 11%
16	BX	28	11% 64% 25% 11%
16	U	28	25% 64% 25% 11%
16	u	28	11% 57% 32% 11%
17	A0	54	6% 67% 33%
17	BY	54	9% 89% 11%
17	W	54	6% 67% 31% •
17	w	54	9% 89% 9% •
18	BA	42	• 69% 17% 14%
18	BZ	42	10% 67% 19% 14%
18	X	42	5% 67% 19% 14%
18	x	42	10% 71% 14% 14%
19	BC	62	• 66% 34%
19	Bb	62	• 66% 34%
19	Z	62	• 65% 35%

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Mol	Chain	Length	Quality of chain
19	z	62	63% 37%
20	A	352	77% 14% 8%
20	BD	352	72% 19% 8%
20	R	352	77% 15% 8%
20	a	352	75% 16% 8%
21	1	459	78% 17% 6%
21	BF	459	9% 77% 17% 6%
21	C	459	77% 17% 6%
21	c	459	9% 76% 18% 6%
22	BU	250	50% 29% 21%
22	r	250	44% 35% 21%

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 146846 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	5	201	1529	991	249	285	4	0	0
1	7	201	1530	991	249	285	5	0	0
1	9	201	1529	991	249	285	4	0	0
1	AA	201	1530	991	249	285	5	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	6	222	1716	1120	280	311	5	0	0
2	0	222	1716	1120	280	311	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	8	192	1512	993	245	270	4	0	0
3	AB	192	1512	993	245	270	4	0	0

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	479	3757	2462	636	647	12	0	0
4	b	479	3757	2462	636	647	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	v	479	3757	2462	636	647	12	0	0
4	BE	479	3757	2462	636	647	12	0	0

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	342	2723	1800	445	466	12	0	0
5	d	342	2723	1800	445	466	12	0	0
5	2	342	2723	1800	445	466	12	0	0
5	BG	342	2723	1800	445	466	12	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	66	544	357	88	99	0	0
6	e	66	544	357	88	99	0	0
6	3	66	544	357	88	99	0	0
6	BH	66	544	357	88	99	0	0

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	29	225	147	40	37	1	0	0
7	f	29	225	147	40	37	1	0	0
7	4	29	225	147	40	37	1	0	0
7	BI	29	225	147	40	37	1	0	0

- Molecule 8 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	206	1562	1010	255	292	5	0	0
8	N	202	1536	994	251	286	5	0	0
8	Y	213	1621	1048	266	302	5	0	0
8	g	206	1562	1010	255	292	5	0	0
8	n	202	1536	994	251	286	5	0	0
8	y	213	1621	1048	266	302	5	0	0
8	Au	206	1562	1010	255	292	5	0	0
8	A2	202	1536	994	251	286	5	0	0
8	BB	213	1621	1048	266	302	5	0	0
8	BJ	206	1562	1010	255	292	5	0	0
8	BQ	202	1536	994	251	286	5	0	0
8	Ba	213	1621	1048	266	302	5	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	59	438	289	68	79	2	0	0
9	h	59	438	289	68	79	2	0	0
9	Av	59	438	289	68	79	2	0	0
9	BK	59	438	289	68	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	35	286	195	44	46	1	0	0
10	i	35	286	195	44	46	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Aw	35	286	195	44	46	1	0	0
			Total	C	N	O	S		
10	BL	35	286	195	44	46	1	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	37	302	211	44	46	1	0	0
			Total	C	N	O	S		
11	k	37	302	211	44	46	1	0	0
			Total	C	N	O	S		
11	Ay	37	302	211	44	46	1	0	0
			Total	C	N	O	S		
11	BN	37	302	211	44	46	1	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	35	293	195	45	53	0	0
			Total	C	N	O		
12	l	35	293	195	45	53	0	0
			Total	C	N	O		
12	Az	35	293	195	45	53	0	0
			Total	C	N	O		
12	BO	35	293	195	45	53	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	32	250	173	35	41	1	0	0
			Total	C	N	O	S		
13	m	32	250	173	35	41	1	0	0
			Total	C	N	O	S		
13	A1	32	250	173	35	41	1	0	0
			Total	C	N	O	S		
13	BP	32	250	173	35	41	1	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S	216	1670	1091	272	303	4	0	0
14	s	216	1670	1091	272	303	4	0	0
14	A6	216	1670	1091	272	303	4	0	0
14	BV	216	1670	1091	272	303	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	T	29	239	168	33	37	1	0	0
15	t	29	239	168	33	37	1	0	0
15	A7	29	239	168	33	37	1	0	0
15	BW	29	239	168	33	37	1	0	0

- Molecule 16 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	U	25	195	122	36	34	3	0	0
16	u	25	195	122	36	34	3	0	0
16	A8	25	195	122	36	34	3	0	0
16	BX	25	195	122	36	34	3	0	0

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	54	428	282	61	84	1	0	0
17	w	54	428	282	61	84	1	0	0
17	A0	54	428	282	61	84	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BY	54	428	282	61	84	1	0	0

- Molecule 18 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	X	36	248	162	39	47	0	0
18	x	36	248	162	39	47	0	0
18	BA	36	248	162	39	47	0	0
18	BZ	36	248	162	39	47	0	0

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	62	465	313	69	82	1	0	0
19	z	62	465	313	69	82	1	0	0
19	BC	62	465	313	69	82	1	0	0
19	Bb	62	465	313	69	82	1	0	0

- Molecule 20 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	A	323	2525	1652	415	445	13	0	0
20	a	323	2525	1652	415	445	13	0	0
20	R	323	2525	1652	415	445	13	0	0
20	BD	323	2525	1652	415	445	13	0	0

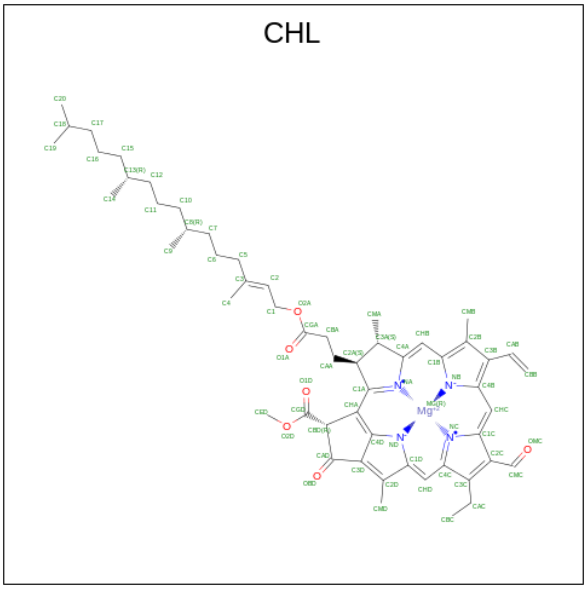
- Molecule 21 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	C	433	3373	2221	563	578	11	0	0
			Total	C	N	O	S		
21	c	432	3365	2217	561	576	11	0	0
			Total	C	N	O	S		
21	1	433	3373	2221	563	578	11	0	0
			Total	C	N	O	S		
21	BF	432	3365	2217	561	576	11	0	0

- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	r	197	1539	1004	251	281	3	0	0
			Total	C	N	O	S		
22	BU	197	1539	1004	251	281	3	0	0

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	5	1	62	51	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	5	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
23	6	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
23	6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	6	1	53	42	1	4	6	0
			Total	C	Mg	N	O	
23	6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	6	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	7	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	7	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	7	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	7	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	7	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	7	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	8	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	8	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	8	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	8	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	G	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	G	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	G	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	G	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	G	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	G	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
23	N	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	N	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	N	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	N	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	N	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	S	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
23	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	Y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Y	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	Y	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	Y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	e	1	45	34	1	4	6	0
			Total	C	Mg	N	O	
23	g	1	65	54	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	g	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	g	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	g	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	g	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	g	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	n	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	n	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	n	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	n	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	n	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	n	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	s	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
23	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	y	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	y	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	y	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	y	1	65	54	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	r	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	r	1	55	44	1	4	6	0
			Total	C	Mg	N	O	
23	r	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	r	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
23	9	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	9	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	9	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	9	1	62	51	1	4	6	0
			Total	C	Mg	N	O	
23	9	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	9	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
23	0	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
23	0	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	0	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	0	1	53	42	1	4	6	0
			Total	C	Mg	N	O	
23	0	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	0	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	AA	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AA	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AA	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AA	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	AA	1	46	35	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	AA	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	AB	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AB	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AB	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AB	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	Au	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Au	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	Au	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	Au	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Au	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Au	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
23	A2	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	A2	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	A2	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	A2	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	A2	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	A2	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	A6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	A6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	A6	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
23	A6	1	46	35	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	BB	1	65	54	1	4	6	0
23	BB	1	48	37	1	4	6	0
23	BB	1	50	39	1	4	6	0
23	BB	1	65	54	1	4	6	0
23	BB	1	65	54	1	4	6	0
23	BB	1	65	54	1	4	6	0
23	BH	1	45	34	1	4	6	0
23	BJ	1	65	54	1	4	6	0
23	BJ	1	46	35	1	4	6	0
23	BJ	1	50	39	1	4	6	0
23	BJ	1	65	54	1	4	6	0
23	BJ	1	65	54	1	4	6	0
23	BJ	1	60	49	1	4	6	0
23	BQ	1	65	54	1	4	6	0
23	BQ	1	48	37	1	4	6	0
23	BQ	1	50	39	1	4	6	0
23	BQ	1	65	54	1	4	6	0
23	BQ	1	65	54	1	4	6	0
23	BQ	1	65	54	1	4	6	0
23	BV	1	46	35	1	4	6	0
23	BV	1	46	35	1	4	6	0

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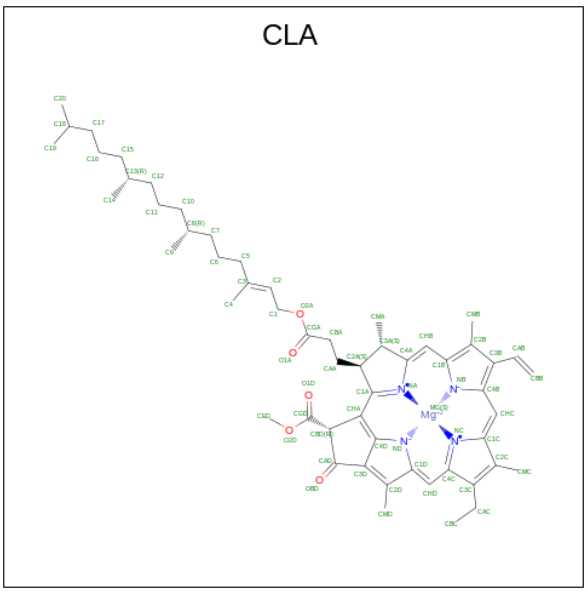
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	BV	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
23	BV	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	Ba	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Ba	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	Ba	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	Ba	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Ba	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	Ba	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	BU	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
23	BU	1	55	44	1	4	6	0
			Total	C	Mg	N	O	
23	BU	1	60	49	1	4	6	0
			Total	C	Mg	N	O	
23	BU	1	42	33	1	4	4	0

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	5	1	61	51	1	4	5	0
24	5	1	55	45	1	4	5	0
24	5	1	50	40	1	4	5	0
24	5	1	56	46	1	4	5	0
24	5	1	45	35	1	4	5	0
24	5	1	45	35	1	4	5	0
24	5	1	55	45	1	4	5	0
24	5	1	45	35	1	4	5	0
24	6	1	60	50	1	4	5	0
24	6	1	55	45	1	4	5	0
24	6	1	45	35	1	4	5	0
24	6	1	60	50	1	4	5	0
24	6	1	55	45	1	4	5	0
24	6	1	45	35	1	4	5	0
24	6	1	58	48	1	4	5	0
24	6	1	48	38	1	4	5	0
24	7	1	61	51	1	4	5	0
24	7	1	55	45	1	4	5	0
24	7	1	45	35	1	4	5	0
24	7	1	48	39	1	4	4	0
24	7	1	45	35	1	4	5	0
24	7	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	N	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	N	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	53	44	1	4	4	0
			Total	C	Mg	N	O	
24	S	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	S	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Y	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	n	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	s	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	y	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	y	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	58	49	1	4	4	0
			Total	C	Mg	N	O	
24	r	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	r	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	r	1	37	31	1	4	1	0
			Total	C	Mg	N	O	
24	r	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	0	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	48	39	1	4	4	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Au	1	48	38	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	Aw	1	65	55	1	4	5	0
24	A2	1	65	55	1	4	5	0
24	A2	1	65	55	1	4	5	0
24	A2	1	50	40	1	4	5	0
24	A2	1	65	55	1	4	5	0
24	A2	1	60	50	1	4	5	0
24	A2	1	60	50	1	4	5	0
24	A2	1	60	50	1	4	5	0
24	A2	1	48	38	1	4	5	0
24	A6	1	61	51	1	4	5	0
24	A6	1	45	35	1	4	5	0
24	A6	1	50	40	1	4	5	0
24	A6	1	45	35	1	4	5	0
24	A6	1	53	44	1	4	4	0
24	A6	1	56	46	1	4	5	0
24	A6	1	49	39	1	4	5	0
24	A6	1	55	45	1	4	5	0
24	A6	1	49	39	1	4	5	0
24	BB	1	65	55	1	4	5	0
24	BB	1	65	55	1	4	5	0
24	BB	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	BB	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BB	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BB	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BB	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BE	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	BG	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BG	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BJ	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	BQ	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	BV	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	BV	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Ba	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	R	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	1	1	65	55	1	4	5	0
24	BD	1	65	55	1	4	5	0
24	BD	1	65	55	1	4	5	0
24	BD	1	50	40	1	4	5	0
24	BD	1	60	50	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0

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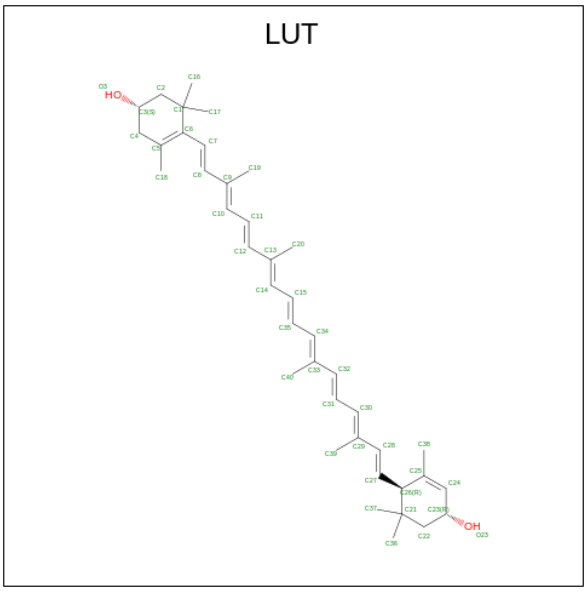
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BF	1	65	55	1	4	5	0
24	BU	1	49	39	1	4	5	0
24	BU	1	58	49	1	4	4	0
24	BU	1	60	50	1	4	5	0
24	BU	1	48	38	1	4	5	0
24	BU	1	58	48	1	4	5	0
24	BU	1	65	55	1	4	5	0
24	BU	1	49	39	1	4	5	0
24	BU	1	49	39	1	4	5	0
24	BU	1	37	31	1	4	1	0
24	BU	1	45	35	1	4	5	0

- Molecule 25 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	5	1	42	40	2	0
			Total	C	O	
25	5	1	42	40	2	0
			Total	C	O	
25	6	1	42	40	2	0
			Total	C	O	
25	6	1	42	40	2	0
			Total	C	O	
25	7	1	42	40	2	0
			Total	C	O	
25	7	1	42	40	2	0
			Total	C	O	
25	8	1	42	40	2	0
			Total	C	O	
25	G	1	42	40	2	0
			Total	C	O	
25	G	1	42	40	2	0
			Total	C	O	
25	N	1	42	40	2	0
			Total	C	O	
25	N	1	42	40	2	0
			Total	C	O	
25	S	1	42	40	2	0
			Total	C	O	
25	S	1	42	40	2	0
			Total	C	O	
25	Y	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	Y	1	42	40	2	0
25	g	1	42	40	2	0
25	g	1	42	40	2	0
25	n	1	42	40	2	0
25	n	1	42	40	2	0
25	s	1	42	40	2	0
25	s	1	42	40	2	0
25	y	1	42	40	2	0
25	y	1	42	40	2	0
25	r	1	42	40	2	0
25	9	1	42	40	2	0
25	9	1	42	40	2	0
25	0	1	42	40	2	0
25	0	1	42	40	2	0
25	AA	1	42	40	2	0
25	AA	1	42	40	2	0
25	AB	1	42	40	2	0
25	Au	1	42	40	2	0
25	Au	1	42	40	2	0
25	A2	1	42	40	2	0
25	A2	1	42	40	2	0

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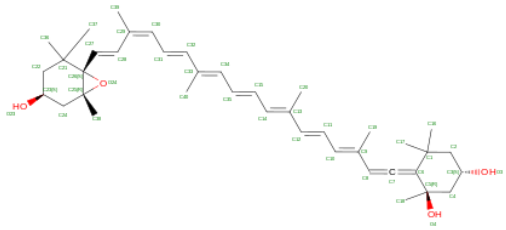
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	A6	1	42	40	2	0
25	A6	1	42	40	2	0
25	BB	1	42	40	2	0
25	BB	1	42	40	2	0
25	BJ	1	42	40	2	0
25	BJ	1	42	40	2	0
25	BQ	1	42	40	2	0
25	BQ	1	42	40	2	0
25	BV	1	42	40	2	0
25	BV	1	42	40	2	0
25	Ba	1	42	40	2	0
25	Ba	1	42	40	2	0
25	BU	1	42	40	2	0

- Molecule 26 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: $C_{40}H_{56}O_4$).

NEX



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	5	1	44	40	4	0
26	7	1	44	40	4	0
26	G	1	44	40	4	0
26	N	1	44	40	4	0
26	S	1	44	40	4	0
26	Y	1	44	40	4	0
26	g	1	44	40	4	0
26	n	1	44	40	4	0
26	s	1	44	40	4	0
26	y	1	44	40	4	0
26	r	1	44	40	4	0
26	9	1	44	40	4	0
26	AA	1	44	40	4	0
26	Au	1	44	40	4	0

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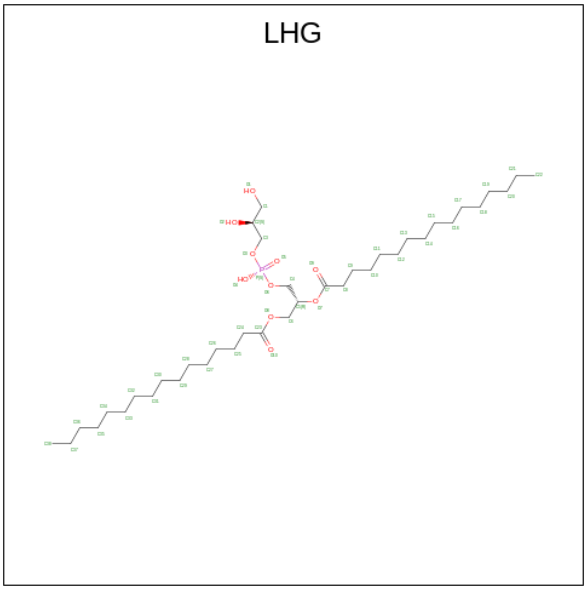
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
26	A2	1	44	40	4		0
26	A6	1	44	40	4		0
26	BB	1	44	40	4		0
26	BB	1	44	40	4		0
26	BJ	1	44	40	4		0
26	BQ	1	44	40	4		0
26	BV	1	44	40	4		0
26	Ba	1	44	40	4		0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	5	1	41	30	10	1	0
27	6	1	47	36	10	1	0
27	B	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	B	1	46	35	10	1	0
27	D	1	49	38	10	1	0
27	G	1	49	38	10	1	0
27	L	1	49	38	10	1	0
27	N	1	49	38	10	1	0
27	W	1	49	38	10	1	0
27	Y	1	49	38	10	1	0
27	b	1	49	38	10	1	0
27	b	1	46	35	10	1	0
27	b	1	49	38	10	1	0
27	d	1	49	38	10	1	0
27	g	1	49	38	10	1	0
27	n	1	49	38	10	1	0
27	w	1	49	38	10	1	0
27	y	1	49	38	10	1	0
27	C	1	49	38	10	1	0
27	C	1	49	38	10	1	0
27	c	1	49	38	10	1	0
27	c	1	49	38	10	1	0
27	r	1	42	31	10	1	0
27	9	1	41	30	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	0	1	47	36	10	1	0
27	v	1	49	38	10	1	0
27	2	1	46	35	10	1	0
27	2	1	49	38	10	1	0
27	Au	1	49	38	10	1	0
27	Az	1	49	38	10	1	0
27	A2	1	49	38	10	1	0
27	A0	1	49	38	10	1	0
27	BB	1	49	38	10	1	0
27	BE	1	49	38	10	1	0
27	BE	1	46	35	10	1	0
27	BE	1	49	38	10	1	0
27	BG	1	49	38	10	1	0
27	BJ	1	49	38	10	1	0
27	BQ	1	49	38	10	1	0
27	BY	1	49	38	10	1	0
27	Ba	1	49	38	10	1	0
27	1	1	49	38	10	1	0
27	1	1	49	38	10	1	0
27	BF	1	49	38	10	1	0
27	BF	1	49	38	10	1	0

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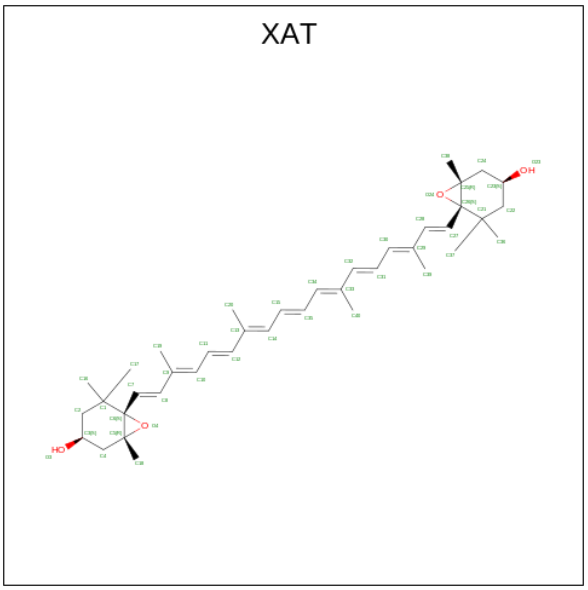
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	BU	1	42	31	10	1	0

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	5	1	44	40	4	0
28	7	1	44	40	4	0
28	7	1	44	40	4	0
28	8	1	44	40	4	0
28	G	1	44	40	4	0
28	N	1	44	40	4	0
28	Y	1	44	40	4	0
28	g	1	44	40	4	0
28	n	1	44	40	4	0
28	y	1	44	40	4	0

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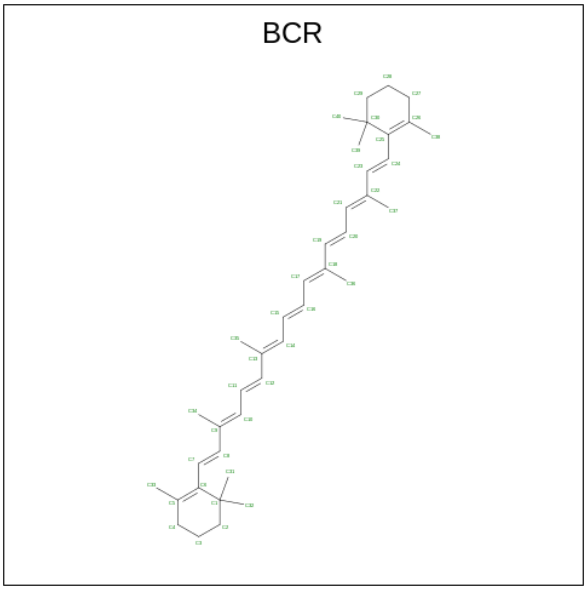
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	r	1	44	40	4	0
28	9	1	44	40	4	0
28	AA	1	44	40	4	0
28	AA	1	44	40	4	0
28	AB	1	44	40	4	0
28	Au	1	44	40	4	0
28	A2	1	44	40	4	0
28	BB	1	44	40	4	0
28	BJ	1	44	40	4	0
28	BQ	1	44	40	4	0
28	Ba	1	44	40	4	0
28	BU	1	44	40	4	0

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
29	8	1	40	40	0
			Total	C	
29	B	1	40	40	0
			Total	C	
29	B	1	40	40	0
			Total	C	
29	B	1	40	40	0
			Total	C	
29	B	1	40	40	0
			Total	C	
29	F	1	40	40	0
			Total	C	
29	H	1	40	40	0
			Total	C	
29	K	1	40	40	0
			Total	C	
29	K	1	40	40	0
			Total	C	
29	b	1	40	40	0
			Total	C	
29	b	1	40	40	0
			Total	C	
29	b	1	40	40	0
			Total	C	
29	b	1	40	40	0
			Total	C	
29	f	1	40	40	0
			Total	C	
29	h	1	40	40	0
			Total	C	
29	k	1	40	40	0
			Total	C	
29	z	1	40	40	0
			Total	C	
29	z	1	40	40	0
			Total	C	
29	A	1	40	40	0
			Total	C	
29	C	1	40	40	0
			Total	C	
29	C	1	40	40	0
			Total	C	
29	a	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
29	c	1	40	40	0
29	AB	1	40	40	0
29	v	1	40	40	0
29	v	1	40	40	0
29	v	1	40	40	0
29	v	1	40	40	0
29	4	1	40	40	0
29	Av	1	40	40	0
29	Ay	1	40	40	0
29	Ay	1	40	40	0
29	BE	1	40	40	0
29	BE	1	40	40	0
29	BE	1	40	40	0
29	BE	1	40	40	0
29	BI	1	40	40	0
29	BK	1	40	40	0
29	BN	1	40	40	0
29	Bb	1	40	40	0
29	R	1	40	40	0
29	1	1	40	40	0
29	1	1	40	40	0

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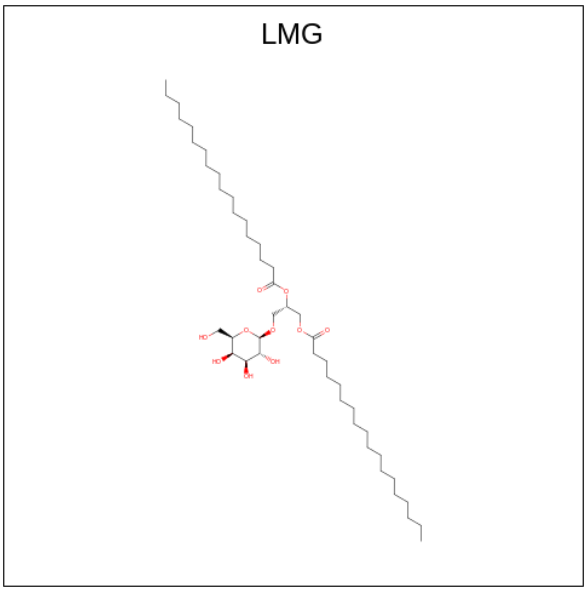
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
29	BD	1	40	40	0
			Total	C	
29	BF	1	40	40	0
			Total	C	
29	BF	1	40	40	0

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	51	41	10	0
			Total	C	O	
30	B	1	40	30	10	0
			Total	C	O	
30	D	1	46	36	10	0
			Total	C	O	
30	I	1	40	30	10	0
			Total	C	O	
30	b	1	51	41	10	0
			Total	C	O	
30	d	1	46	36	10	0
			Total	C	O	
30	i	1	48	38	10	0
			Total	C	O	
30	A	1	48	38	10	0

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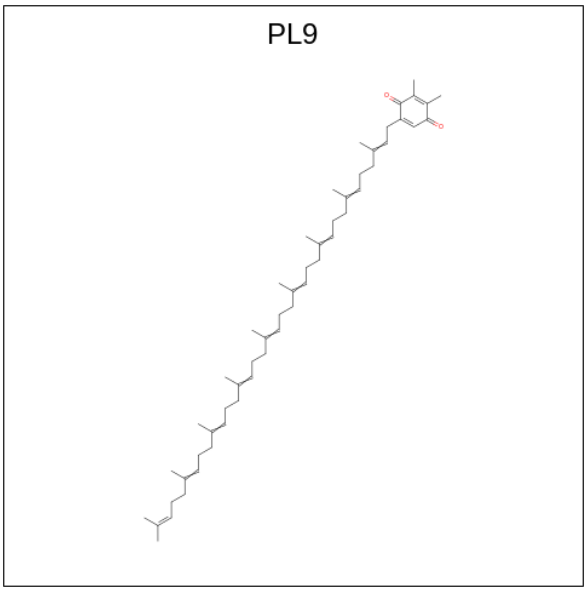
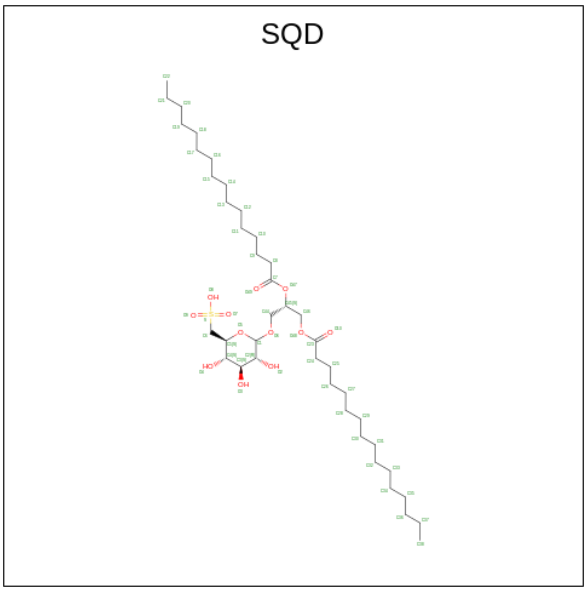
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	C	1	51	41	10	0
			Total	C	O	
30	C	1	51	41	10	0
			Total	C	O	
30	c	1	51	41	10	0
			Total	C	O	
30	c	1	51	41	10	0
			Total	C	O	
30	v	1	51	41	10	0
			Total	C	O	
30	v	1	40	30	10	0
			Total	C	O	
30	2	1	46	36	10	0
			Total	C	O	
30	Aw	1	40	30	10	0
			Total	C	O	
30	A0	1	48	38	10	0
			Total	C	O	
30	BE	1	51	41	10	0
			Total	C	O	
30	BG	1	46	36	10	0
			Total	C	O	
30	BL	1	48	38	10	0
			Total	C	O	
30	1	1	51	41	10	0
			Total	C	O	
30	1	1	51	41	10	0
			Total	C	O	
30	BF	1	51	41	10	0
			Total	C	O	
30	BF	1	51	41	10	0

- Molecule 31 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: $C_{53}H_{80}O_2$).



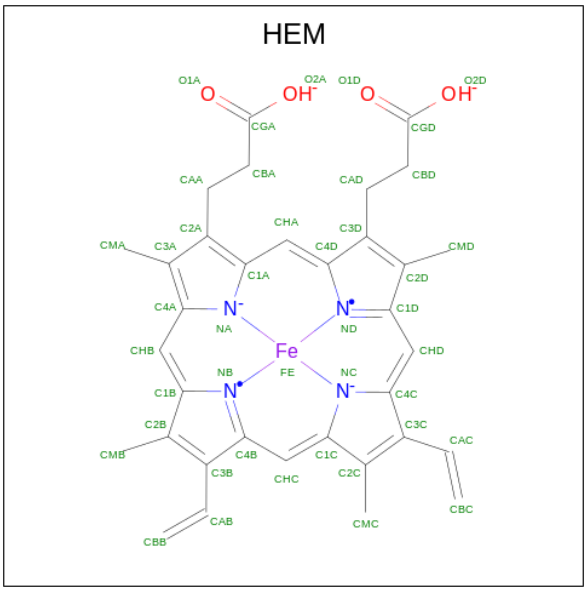
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	D	1	55	53	2	0
31	d	1	55	53	2	0
31	2	1	55	53	2	0
31	BG	1	55	53	2	0

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



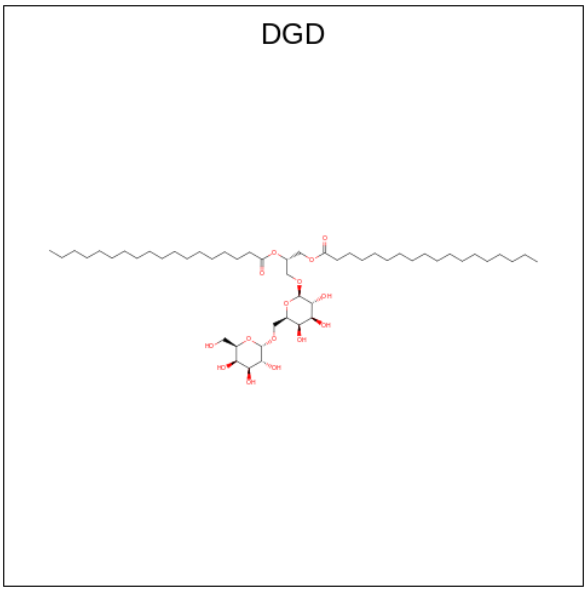
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	D	1	50	37	12	1	0
32	L	1	42	29	12	1	0
32	L	1	54	41	12	1	0
32	d	1	50	37	12	1	0
32	l	1	54	41	12	1	0
32	l	1	42	29	12	1	0
32	A	1	54	41	12	1	0
32	a	1	54	41	12	1	0
32	2	1	50	37	12	1	0
32	Az	1	42	29	12	1	0
32	A1	1	54	41	12	1	0
32	BG	1	50	37	12	1	0
32	BO	1	54	41	12	1	0
32	BO	1	42	29	12	1	0
32	R	1	54	41	12	1	0
32	BD	1	54	41	12	1	0

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



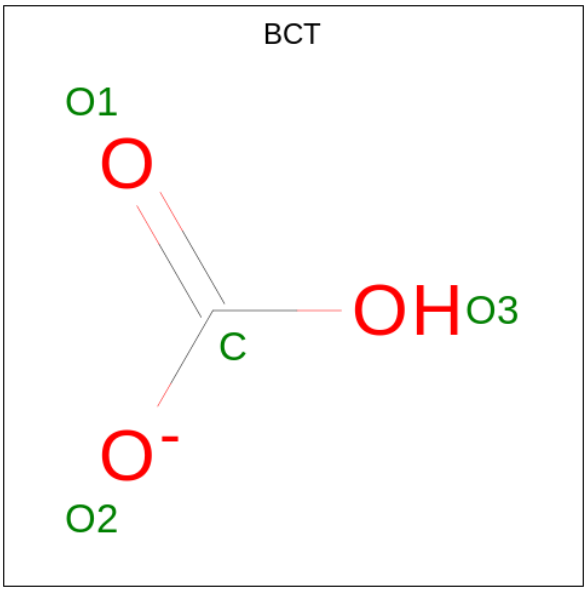
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
33	F	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
33	f	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
33	4	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
33	BI	1	43	34	1	4	4	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



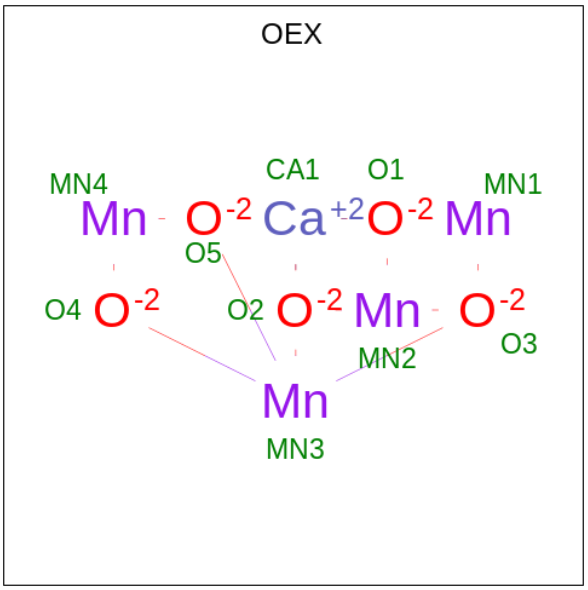
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	H	1	62	47	15	0
34	h	1	62	47	15	0
34	A	1	59	44	15	0
34	C	1	55	40	15	0
34	C	1	62	47	15	0
34	C	1	60	45	15	0
34	a	1	59	44	15	0
34	a	1	60	45	15	0
34	c	1	55	40	15	0
34	c	1	62	47	15	0
34	Av	1	62	47	15	0
34	BK	1	62	47	15	0
34	R	1	59	44	15	0
34	1	1	55	40	15	0
34	1	1	62	47	15	0
34	1	1	60	45	15	0
34	BD	1	59	44	15	0
34	BD	1	60	45	15	0
34	BF	1	55	40	15	0
34	BF	1	62	47	15	0

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	A	1	4	1	3	0
35	a	1	4	1	3	0
35	2	1	4	1	3	0
35	BD	1	4	1	3	0

- Molecule 36 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

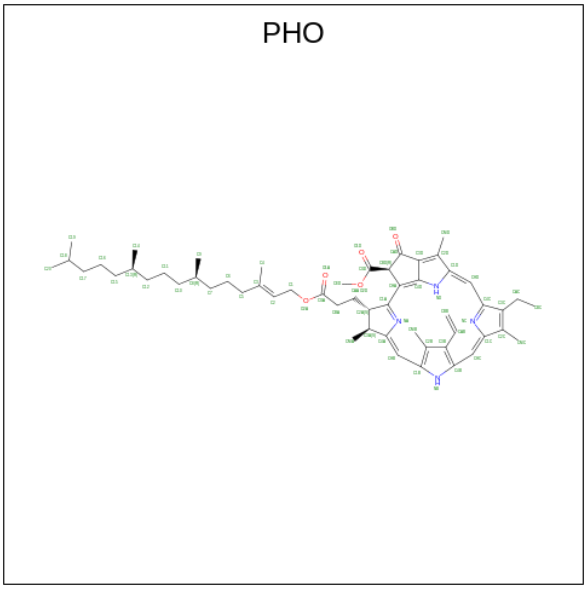


Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
36	A	1	10	1	4	5	0
36	a	1	10	1	4	5	0
36	R	1	10	1	4	5	0
36	BD	1	10	1	4	5	0

- Molecule 37 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
37	A	1	1	1	0
37	a	1	1	1	0
37	R	1	1	1	0
37	BD	1	1	1	0

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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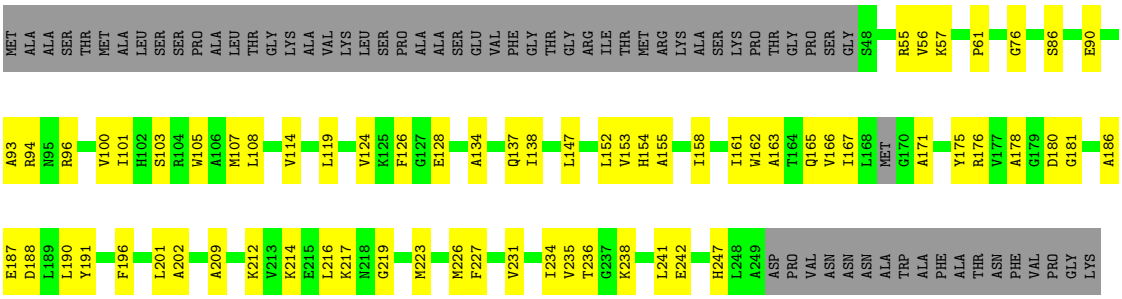
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
38	a	1	64	55	4	5	0
38	a	1	64	55	4	5	0
38	R	1	64	55	4	5	0
38	R	1	64	55	4	5	0
38	BD	1	64	55	4	5	0
38	BD	1	64	55	4	5	0

3 Residue-property plots (i)

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

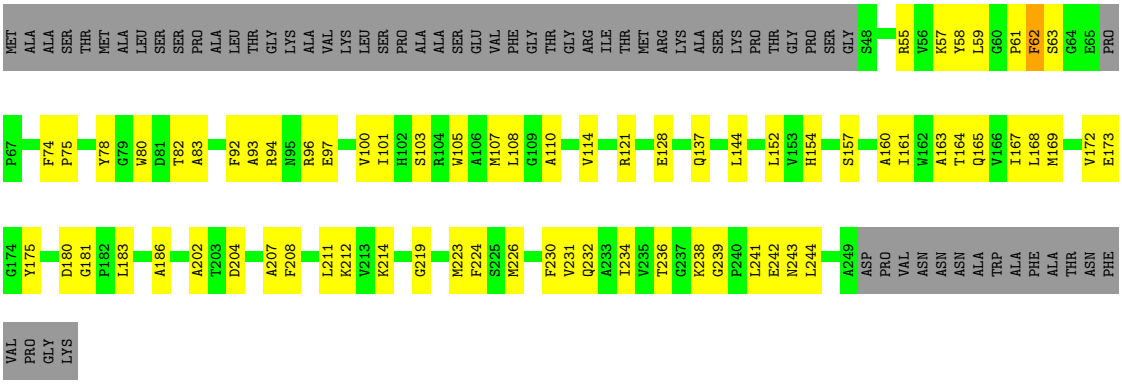
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 50% 25% 24%



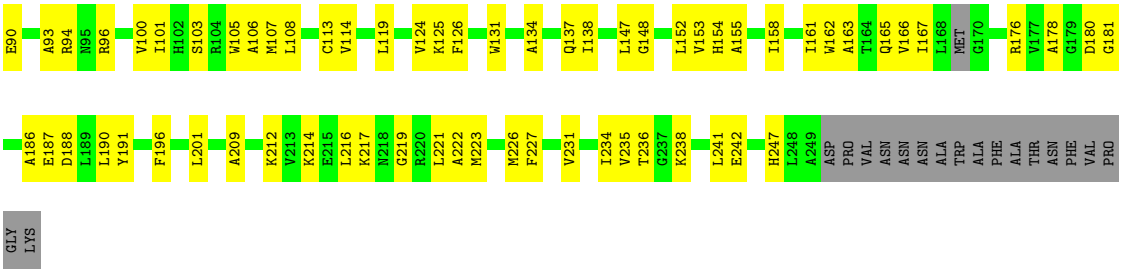
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 49% 26% 24%



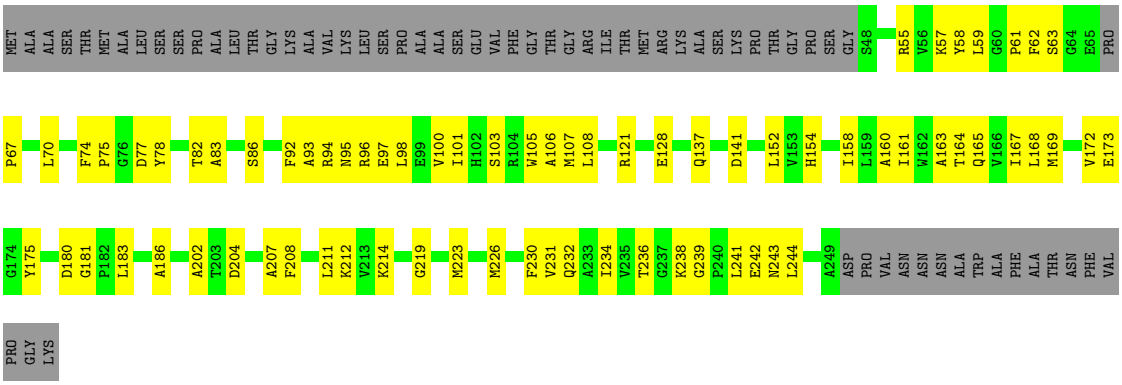
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 9: 49% 27% 24%



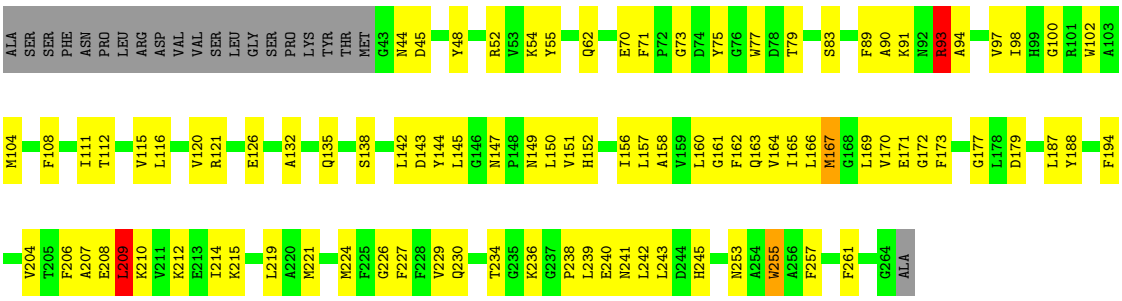
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain AA: 48% 27% 24%



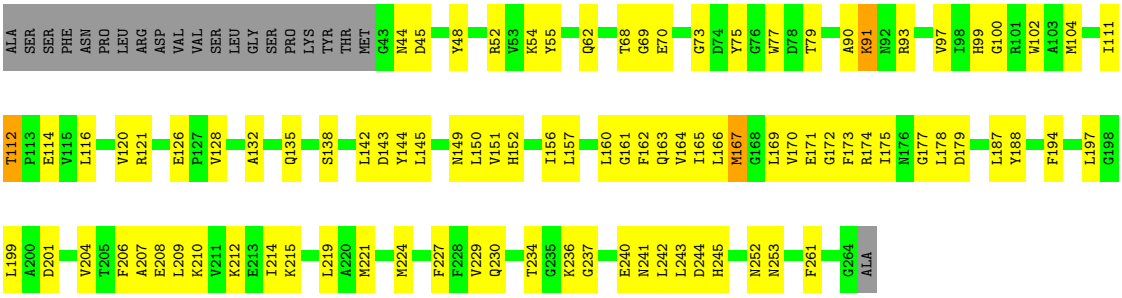
• Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

Chain 6: 53% 37% •• 9%



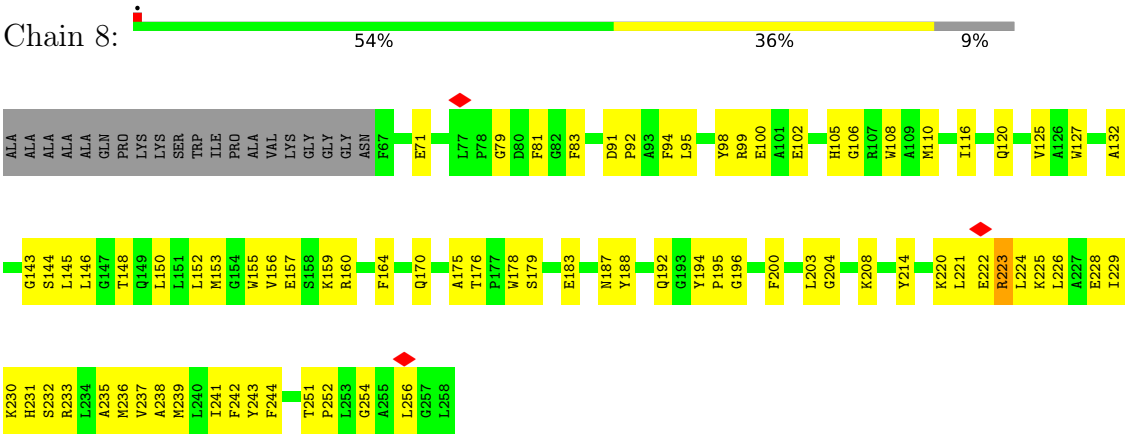
• Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

Chain 0: 53% 37% • 9%



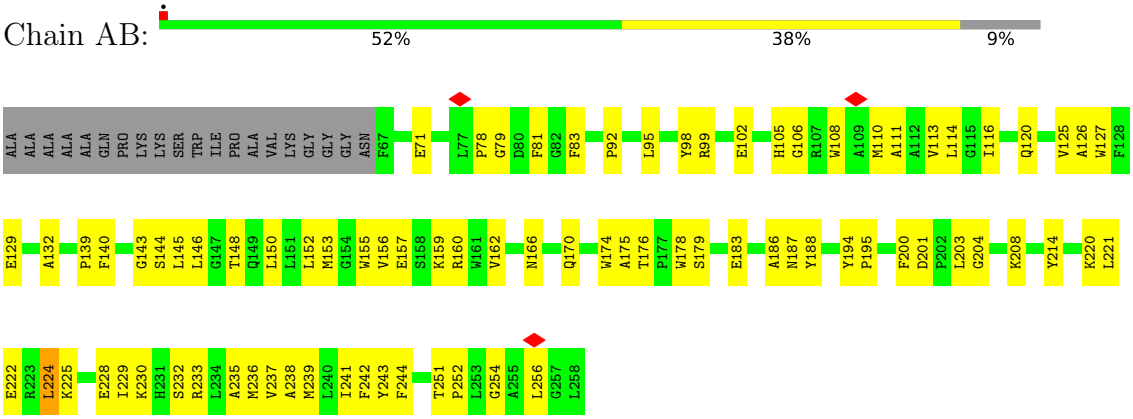
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



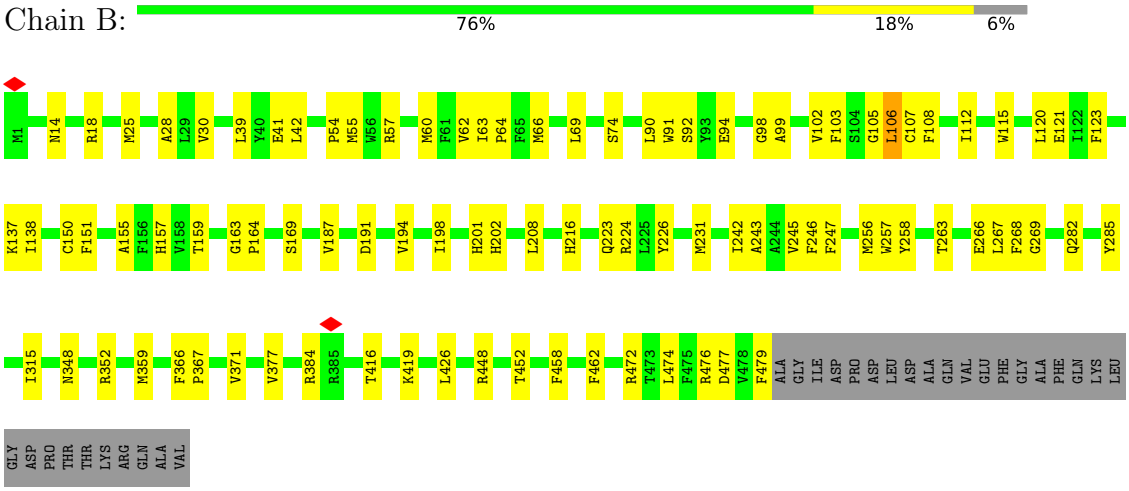
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain AB:



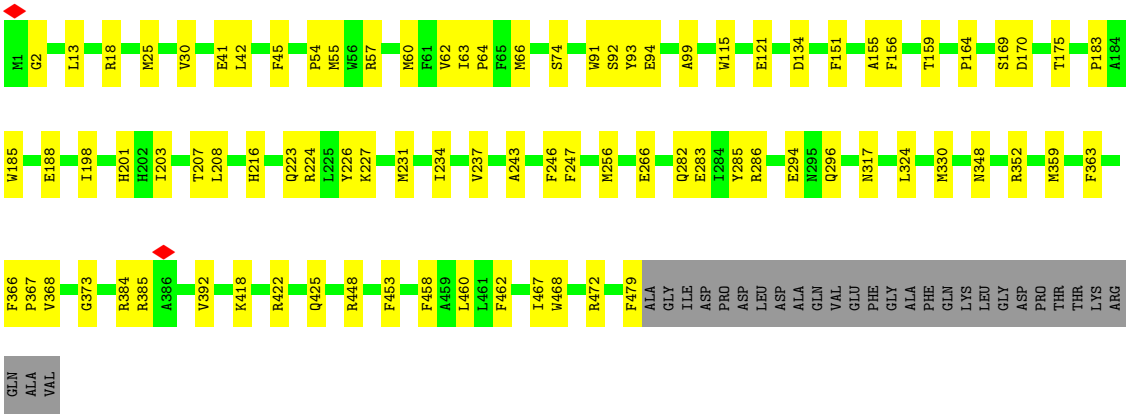
• Molecule 4: Photosystem II CP47 reaction center protein

Chain B:



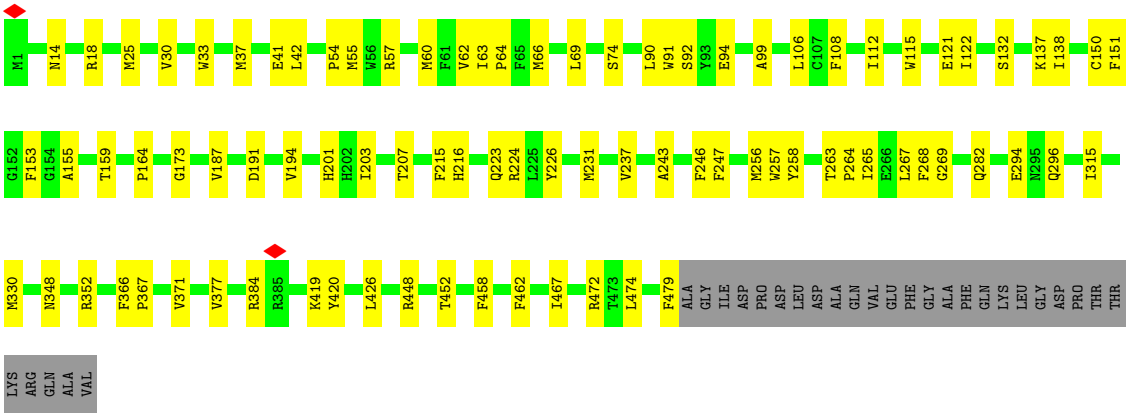
• Molecule 4: Photosystem II CP47 reaction center protein

Chain b:



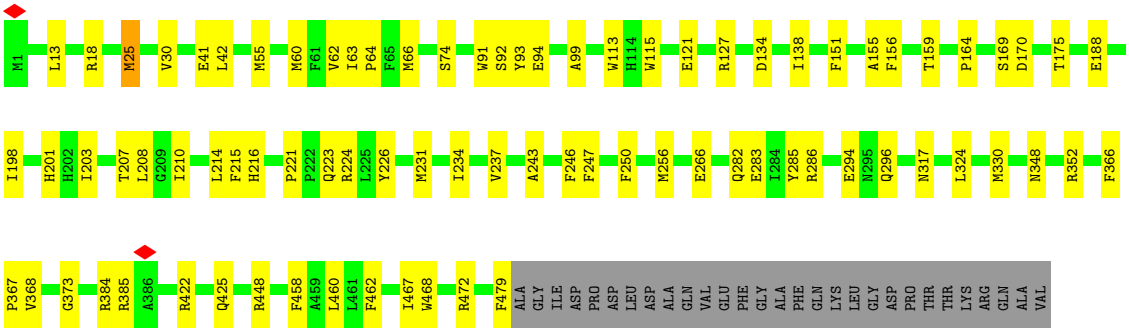
• Molecule 4: Photosystem II CP47 reaction center protein

Chain v:



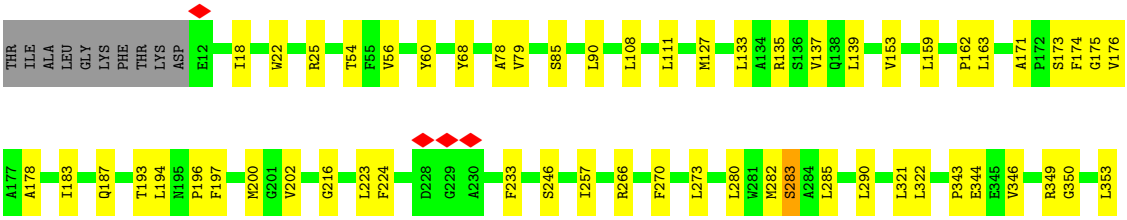
• Molecule 4: Photosystem II CP47 reaction center protein

Chain BE:



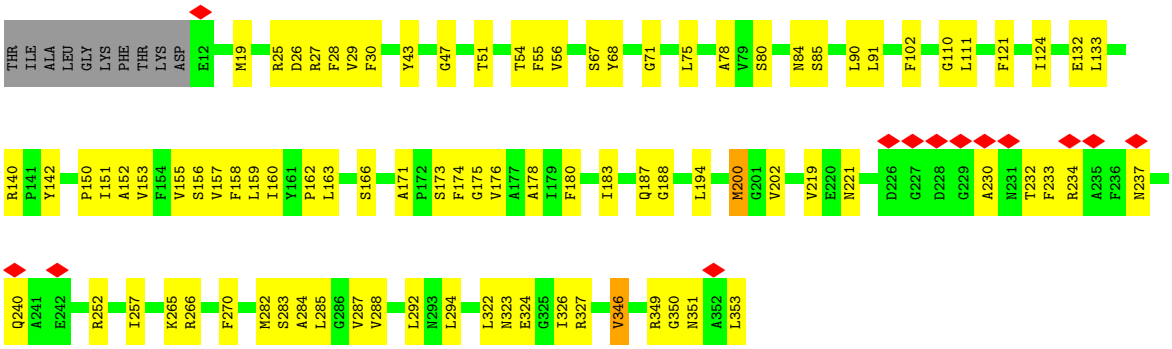
• Molecule 5: Photosystem II D2 protein

Chain D:



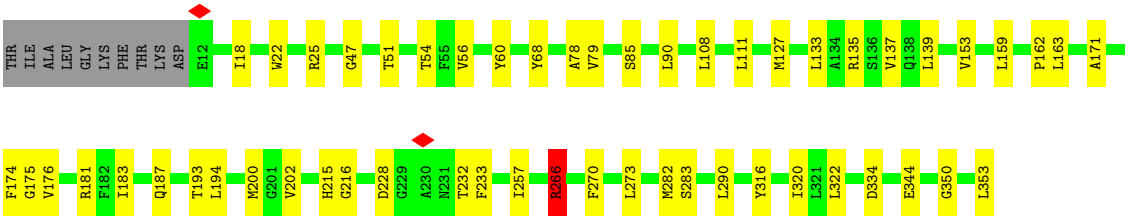
• Molecule 5: Photosystem II D2 protein

Chain d:



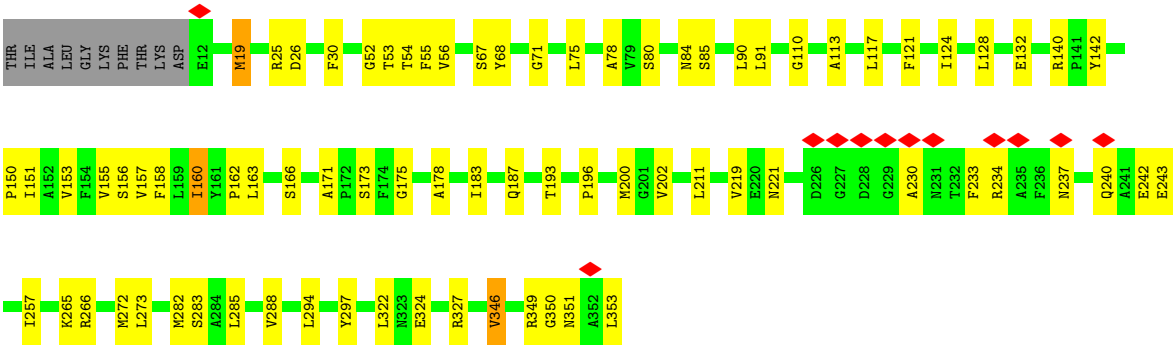
• Molecule 5: Photosystem II D2 protein

Chain 2:



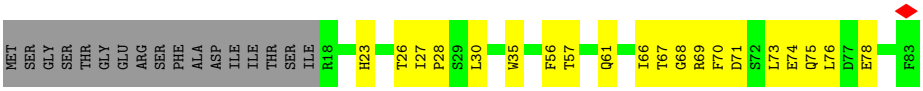
• Molecule 5: Photosystem II D2 protein

Chain BG:



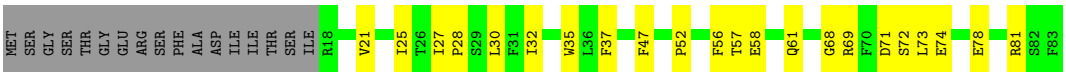
• Molecule 6: Cytochrome b559 subunit alpha

Chain E:



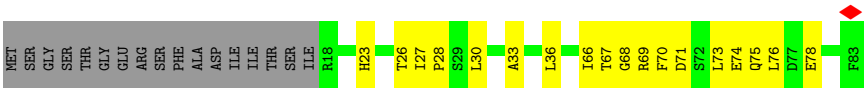
• Molecule 6: Cytochrome b559 subunit alpha

Chain e:



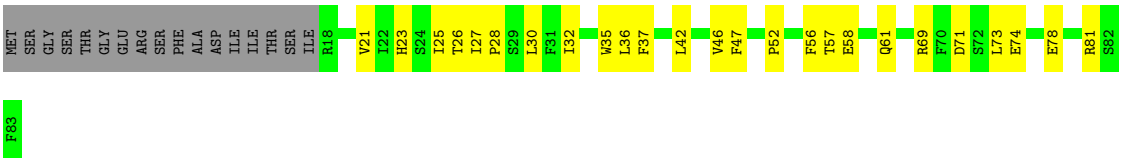
• Molecule 6: Cytochrome b559 subunit alpha

Chain 3:



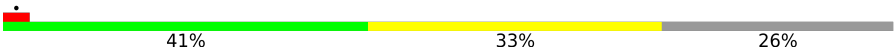
• Molecule 6: Cytochrome b559 subunit alpha

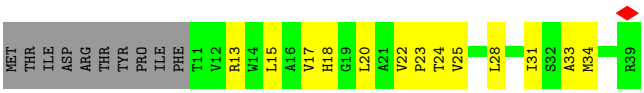
Chain BH:



• Molecule 7: Cytochrome b559 subunit beta

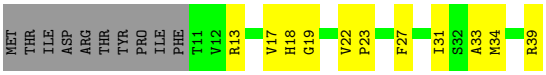
Chain F:





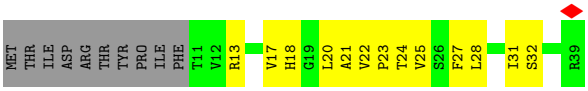
• Molecule 7: Cytochrome b559 subunit beta

Chain f:



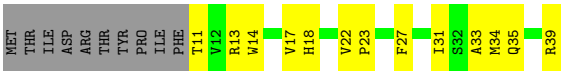
• Molecule 7: Cytochrome b559 subunit beta

Chain 4:



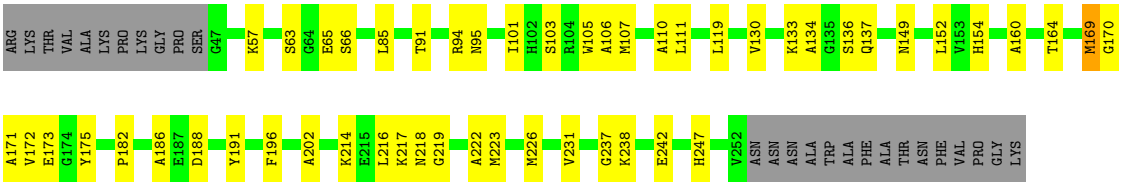
• Molecule 7: Cytochrome b559 subunit beta

Chain BI: 41% 33% 26%



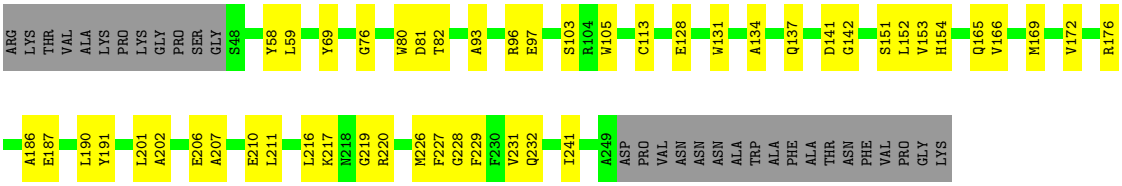
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain G: 67% 22% 11%



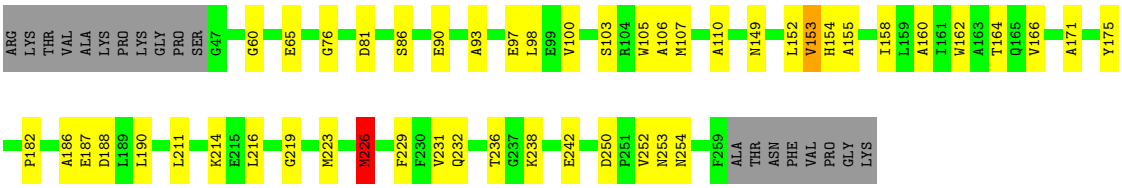
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain N: 66% 21% 13%



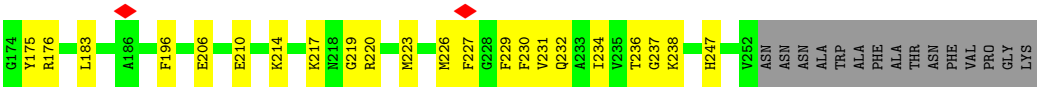
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain Y: 71% 20% 8%



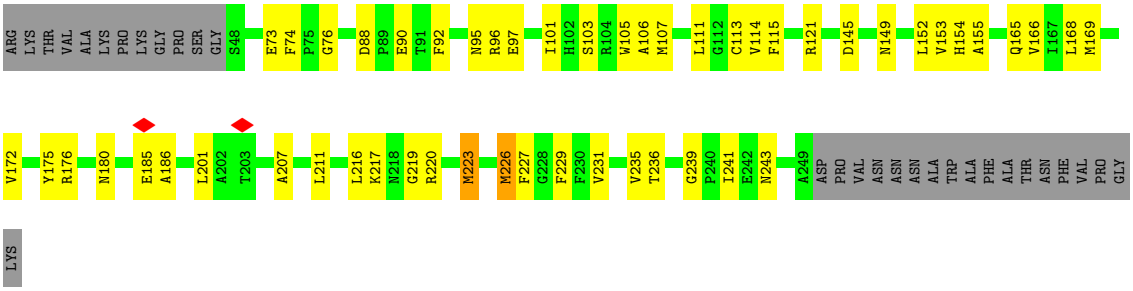
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain g: 69% 20% 11%



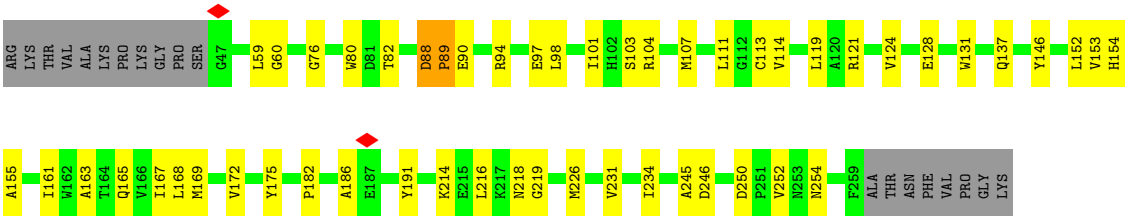
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain n:



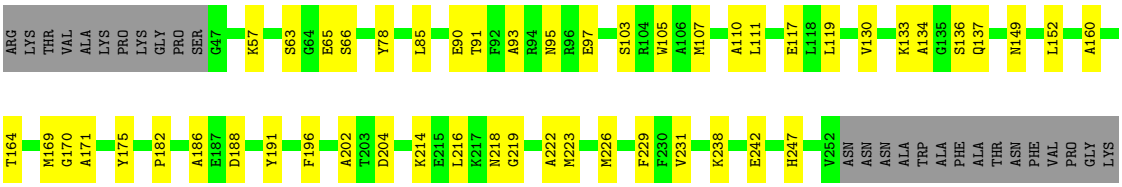
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain y:



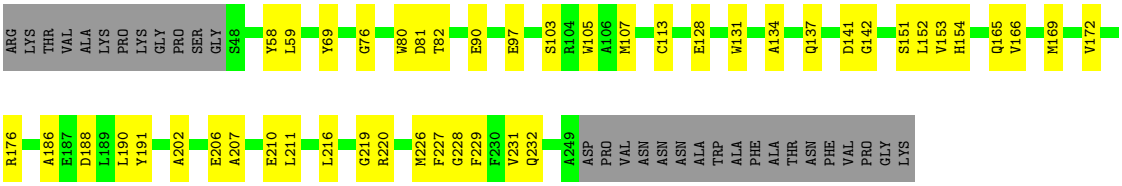
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain Au:



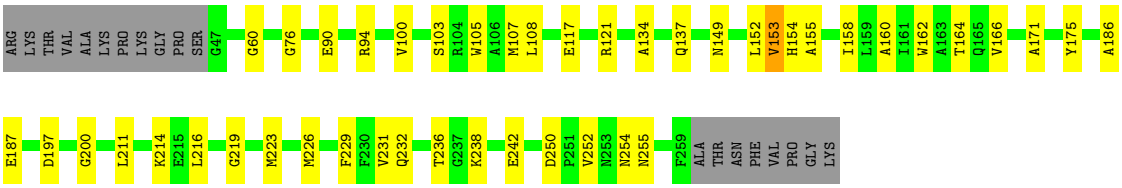
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain A2:



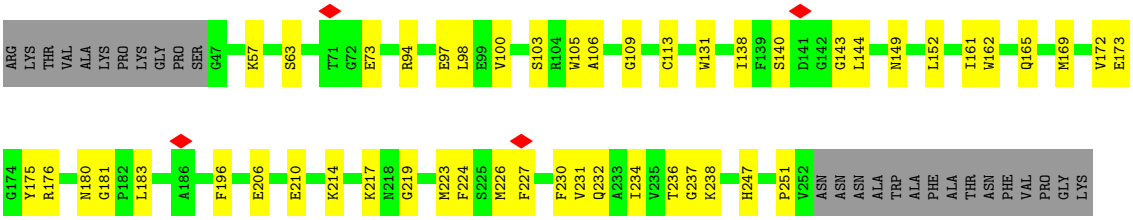
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BB: 72% 19% 8%



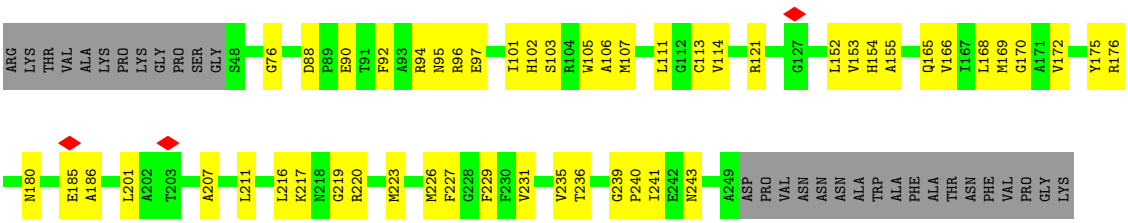
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BJ: 68% 21% 11%



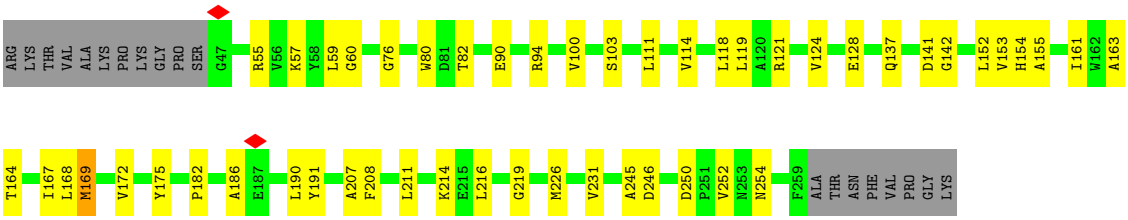
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BQ: 65% 22% 13%



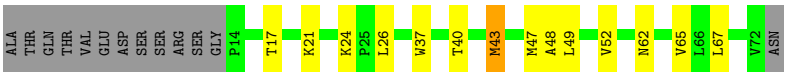
• Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain Ba: 70% 21% 8%



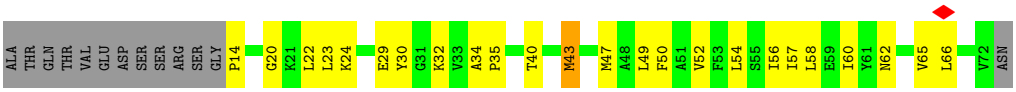
• Molecule 9: Photosystem II reaction center protein H

Chain H: 62% 18% • 18%



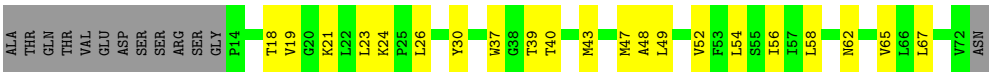
• Molecule 9: Photosystem II reaction center protein H

Chain h:



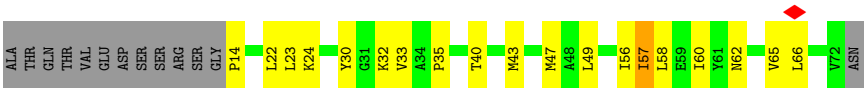
• Molecule 9: Photosystem II reaction center protein H

Chain Av:



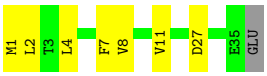
• Molecule 9: Photosystem II reaction center protein H

Chain BK:



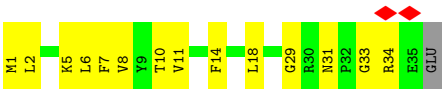
• Molecule 10: Photosystem II reaction center protein I

Chain I:



• Molecule 10: Photosystem II reaction center protein I

Chain i:

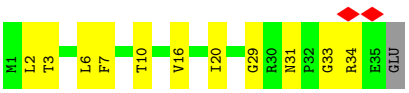


• Molecule 10: Photosystem II reaction center protein I

Chain Aw:

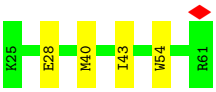
• Molecule 10: Photosystem II reaction center protein I

Chain BL:



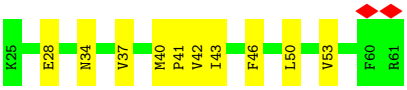
• Molecule 11: Photosystem II reaction center protein K

Chain K:



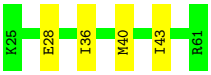
• Molecule 11: Photosystem II reaction center protein K

Chain k:



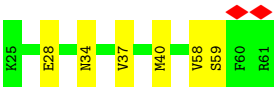
• Molecule 11: Photosystem II reaction center protein K

Chain Ay:



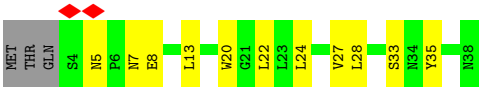
• Molecule 11: Photosystem II reaction center protein K

Chain BN:



• Molecule 12: Photosystem II reaction center protein L

Chain L:



• Molecule 12: Photosystem II reaction center protein L

Chain l:

• Molecule 12: Photosystem II reaction center protein L

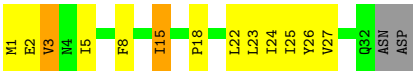
Chain Az:

• Molecule 12: Photosystem II reaction center protein L

Chain BO:

• Molecule 13: Photosystem II reaction center protein M

Chain M:



• Molecule 13: Photosystem II reaction center protein M

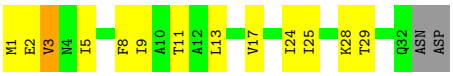
Chain m:

• Molecule 13: Photosystem II reaction center protein M

Chain A1:

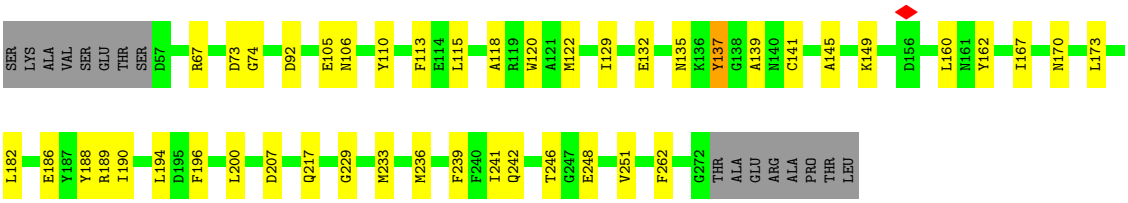
• Molecule 13: Photosystem II reaction center protein M

Chain BP:



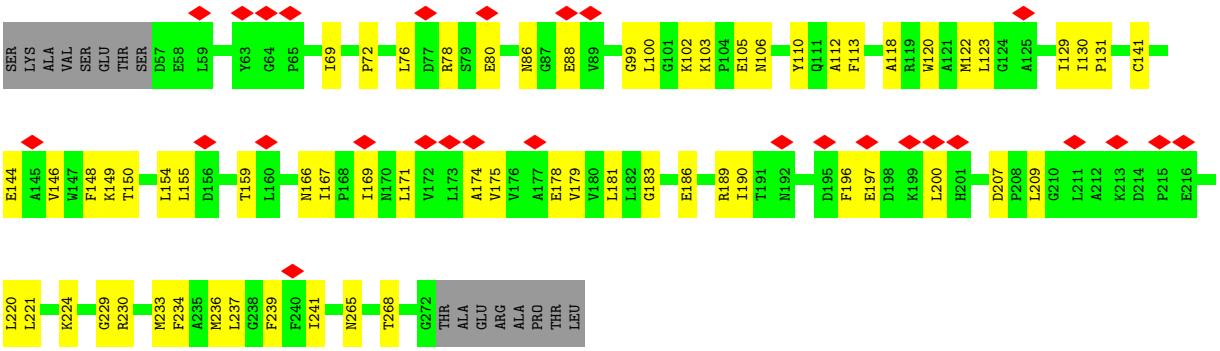
• Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S:



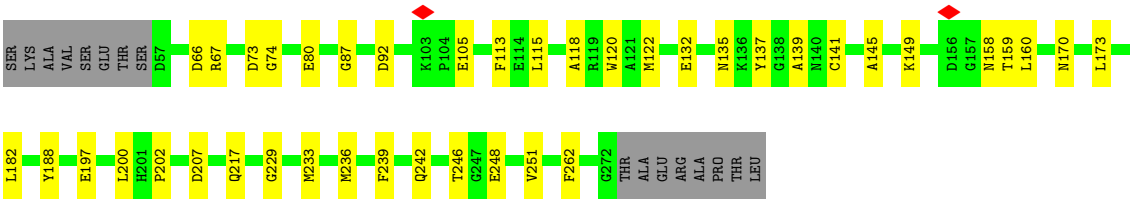
• Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

Chain s:



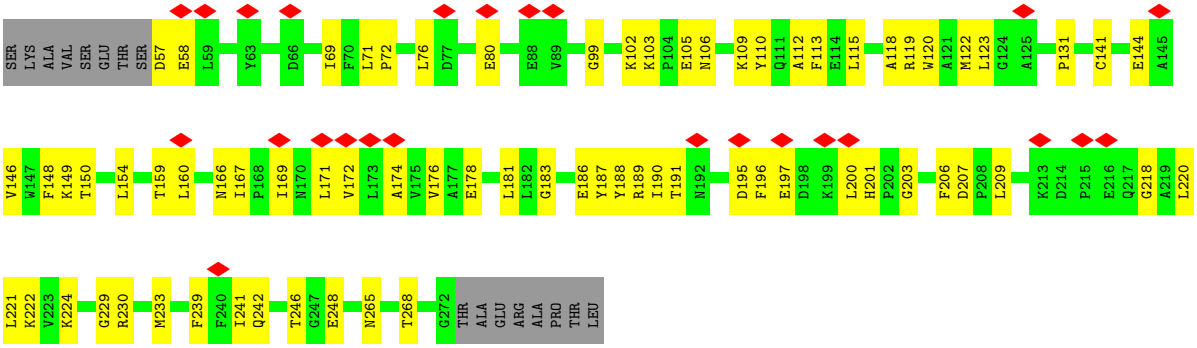
• Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

Chain A6:



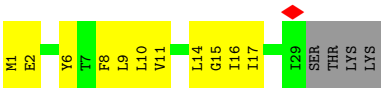
• Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

Chain BV:



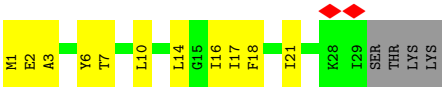
• Molecule 15: Photosystem II reaction center protein T

Chain T:



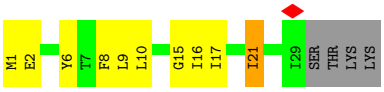
• Molecule 15: Photosystem II reaction center protein T

Chain t:



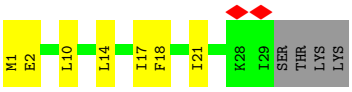
• Molecule 15: Photosystem II reaction center protein T

Chain A7:



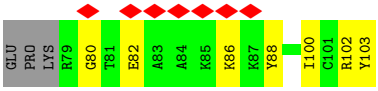
• Molecule 15: Photosystem II reaction center protein T

Chain BW:



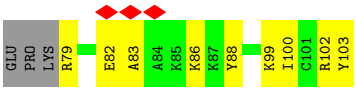
• Molecule 16: Photosystem II 5 kDa protein, chloroplastic

Chain U:



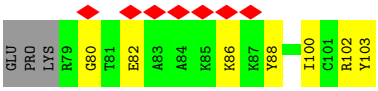
• Molecule 16: Photosystem II 5 kDa protein, chloroplastic

Chain u:



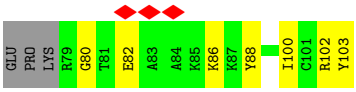
• Molecule 16: Photosystem II 5 kDa protein, chloroplastic

Chain A8:



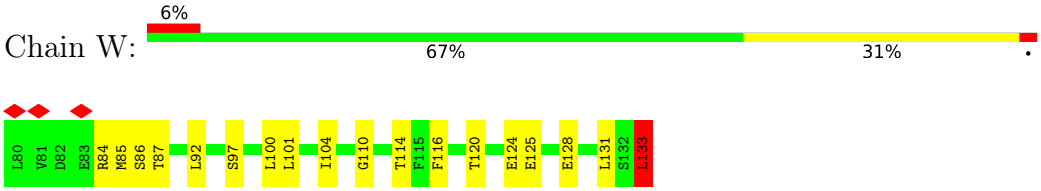
• Molecule 16: Photosystem II 5 kDa protein, chloroplastic

Chain BX:



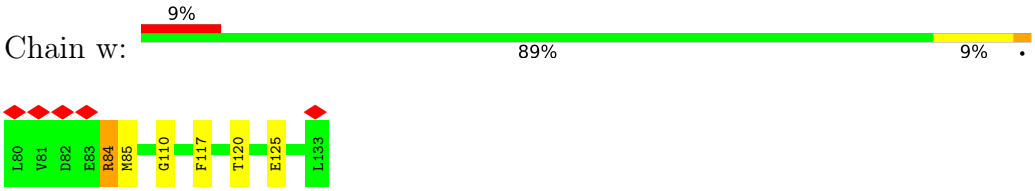
• Molecule 17: Photosystem II reaction center W protein, chloroplastic

Chain W:



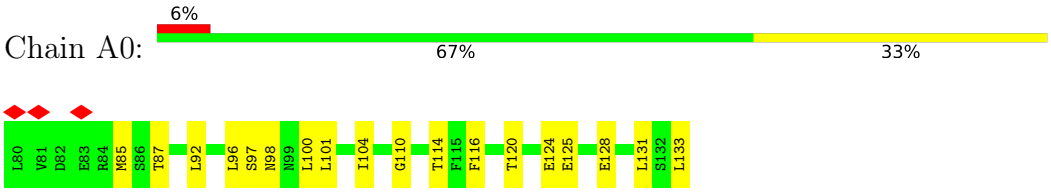
• Molecule 17: Photosystem II reaction center W protein, chloroplastic

Chain w:



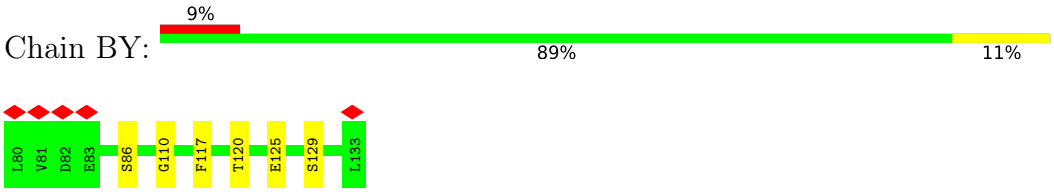
• Molecule 17: Photosystem II reaction center W protein, chloroplastic

Chain A0:



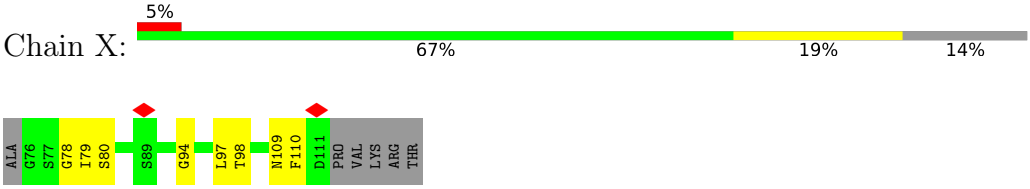
• Molecule 17: Photosystem II reaction center W protein, chloroplastic

Chain BY:



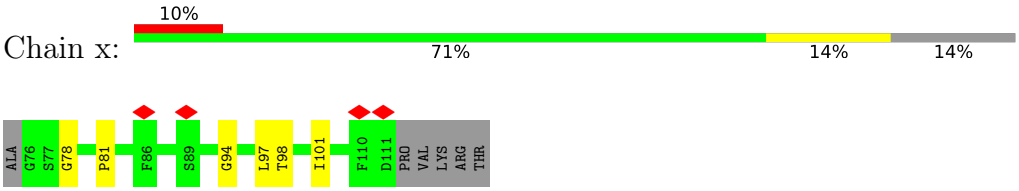
• Molecule 18: (thale cress) hypothetical protein

Chain X:



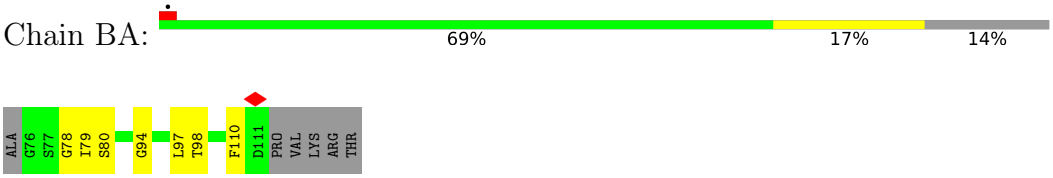
• Molecule 18: (thale cress) hypothetical protein

Chain x:



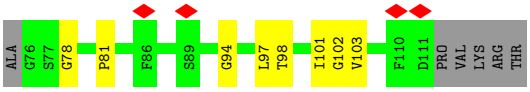
• Molecule 18: (thale cress) hypothetical protein

Chain BA:



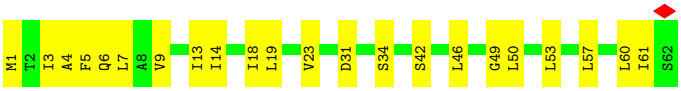
• Molecule 18: (thale cress) hypothetical protein

Chain BZ:



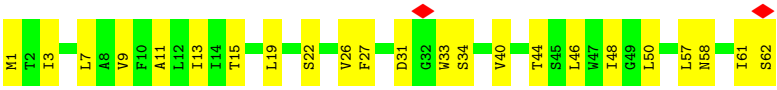
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



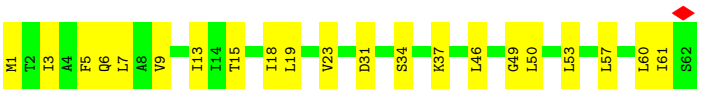
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



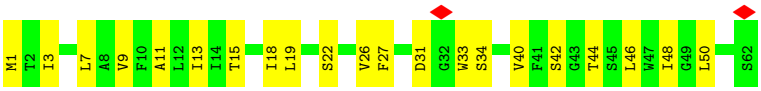
• Molecule 19: Photosystem II reaction center protein Z

Chain BC:



• Molecule 19: Photosystem II reaction center protein Z

Chain Bb:



• Molecule 20: Photosystem II protein D1

Chain A:

• Molecule 20: Photosystem II protein D1

Chain a: 75% 16% 8%

THR ALA ILE LEU GLU ARG ARG GLU SER E11 W20 E25 T43 D61 G62 I63 I77 I82 H92 W97 E98 A99 A100 E104 W105 N108 L120 W131 E132 L133 S134 M139 R140 P141 W142 I143 L159 P162 L174 G175 I176 M183

A188 M199 L200 G201 V202 A203 G204 L223 I224 R225 E226 T227 T228 E229 ASN GLU SER A233 N234 E235 G236 Y237 R238 T245 Y246 N247 I248 F260 A263 S268 R269 S270 L271 H272 W278 I283 W284 F285 T286 A287 L288 D308 R312 M328 M331 H332 E333 R334

N335 A336 HIS ASN PHE PRO LEU ASP LEU ALA ALA VAL GLU ALA PRO SER THR ASN GLY

• Molecule 20: Photosystem II protein D1

Chain R: 77% 15% 8%

THR ALA ILE LEU GLU ARG ARG GLU SER E11 W20 T45 I49 A88 S101 V102 D103 E104 W105 G110 F119 L120 W131 E132 L133 S134 M139 A153 V157 F158 L159 P162 M172 I176 F182 M183 I184 A188 P196 M199 L200 G201

G204 S217 L218 V219 T220 E226 T227 T228 E229 ASN GLU SER A233 N234 E235 G236 Y237 R238 E242 A251 I259 F260 R269 A276 A277 W278 I283 T286 A287 L288 G289 I290 M293 Q304 D308 S309 Q310 G311 R312 M328 R334 N335 A336 HIS ASN

PHE PRO LEU ASP LEU ALA ALA VAL GLU ALA PRO SER THR ASN GLY

• Molecule 20: Photosystem II protein D1

Chain BD: 72% 19% 8%

THR ALA ILE LEU GLU ARG ARG GLU SER E11 W20 M37 I38 L41 I49 I53 D61 I77 I82 H92 E104 N108 L120 W131 E132 L133 S134 M139 I143 L159 P162 L174 G175 I176 M183 F186 I192 L193 M194

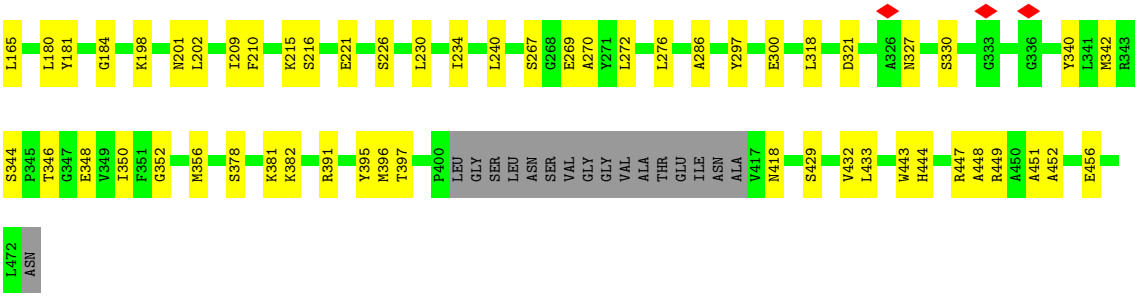
H195 H198 G201 V202 A203 G204 V205 S217 L223 I224 R225 E226 T227 T228 E229 ASN GLU SER A233 N234 E235 G236 Y237 R238 E242 E243 E244 T245 Y246 N247 I248 F260 A263 S268 R269 S270 L271 H272 W278 T286 A287 L288 G289 I290 S291 T292 M293 L297

D308 R312 A324 N325 L326 G327 M328 M331 H332 E333 R334 N335 A336 HIS ASN PHE PRO LEU ASP LEU ALA ALA VAL GLU ALA PRO SER THR ASN GLY

• Molecule 21: Photosystem II CP43 reaction center protein

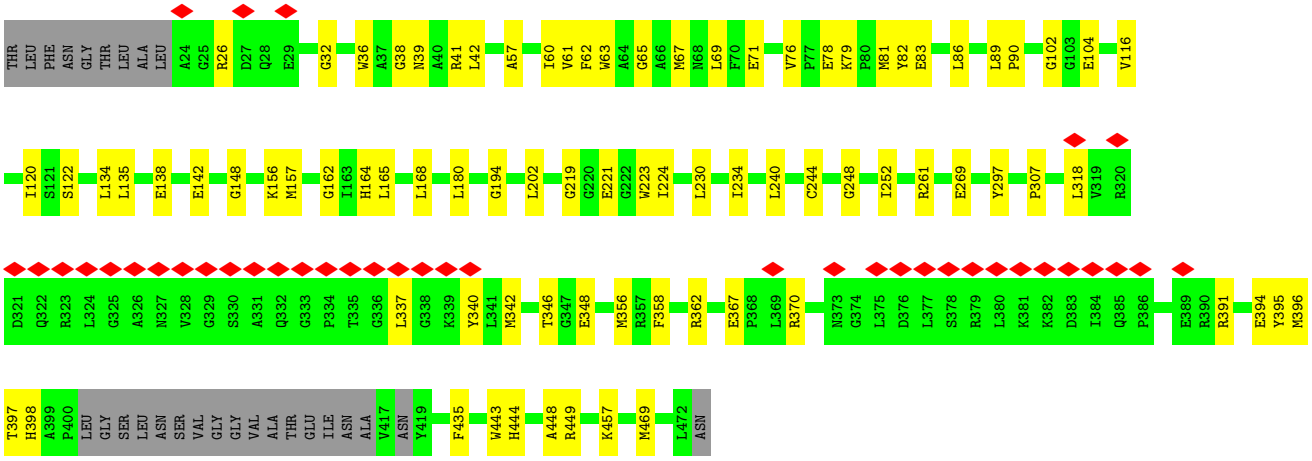
Chain C: 77% 17% 6%

THR LEU PHE ASN GLY THR LEU ALA LEU A24 G25 R26 T31 G32 F33 N39 A40 R41 L42 L45 A55 H56 A57 G58 V61 N68 V76 P77 E78 M81 L86 I87 P90 S122 I130 L134 E138 E142 W151 K152 D153 M157



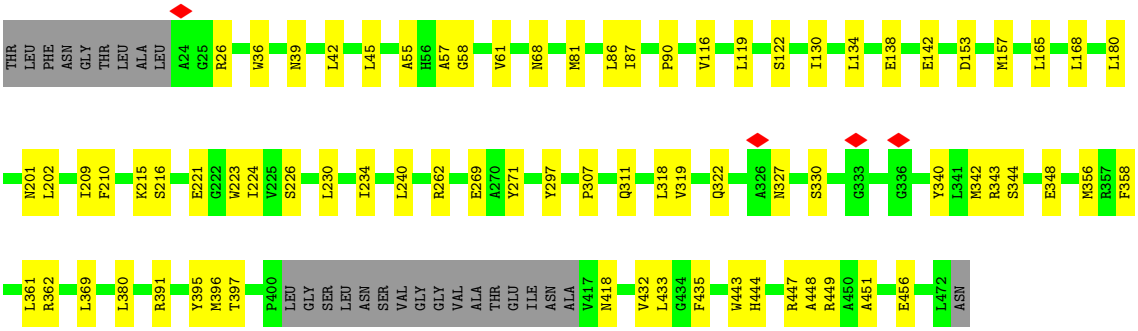
• Molecule 21: Photosystem II CP43 reaction center protein

Chain c:



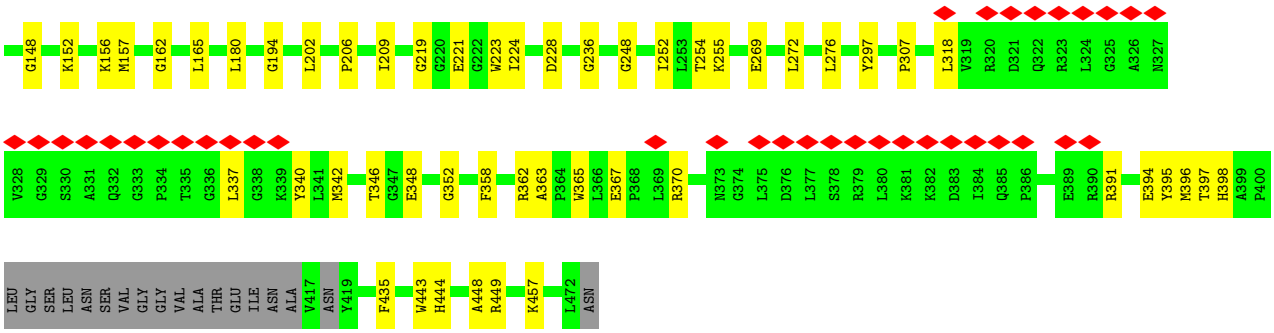
• Molecule 21: Photosystem II CP43 reaction center protein

Chain 1:



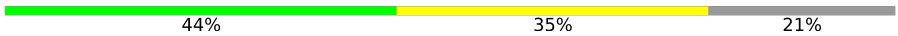
• Molecule 21: Photosystem II CP43 reaction center protein

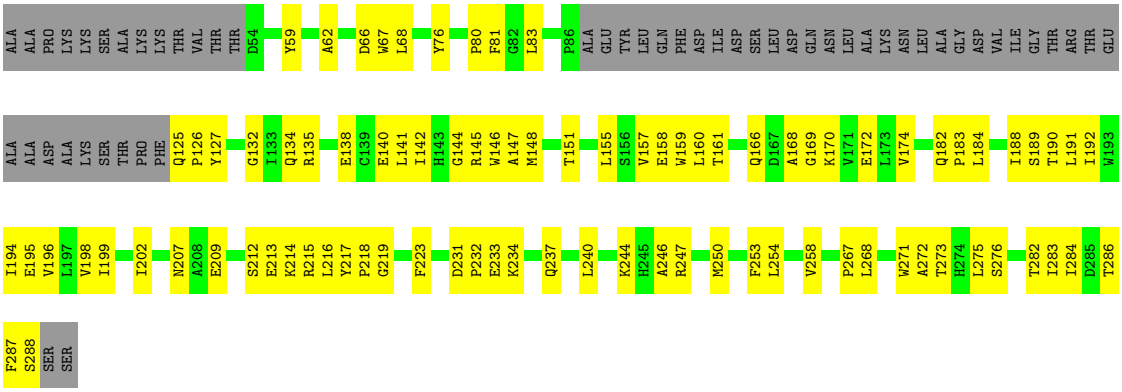
Chain BF:



• Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

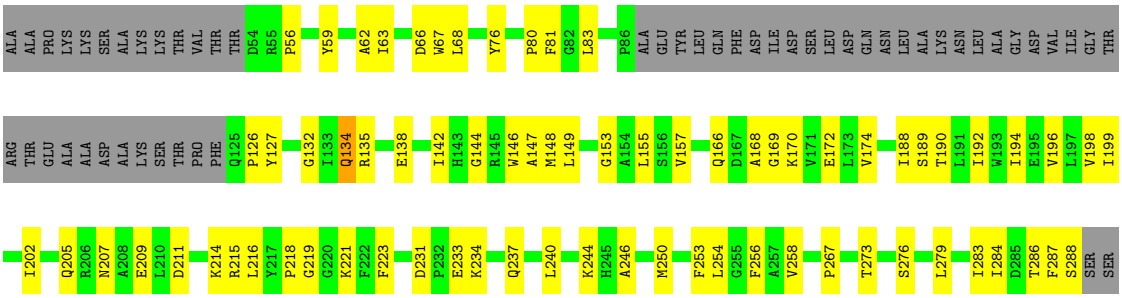
Chain r:





• Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain BU:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.874	Depositor
Minimum map value	-18.604	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	770.4, 770.4, 770.4	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	5	0.26	0/1573	0.44	0/2137
1	7	0.28	0/1573	0.45	0/2134
1	9	0.25	0/1573	0.38	0/2137
1	AA	0.31	0/1573	0.45	0/2134
2	0	0.34	0/1768	0.55	2/2405 (0.1%)
2	6	0.36	0/1768	0.58	3/2405 (0.1%)
3	8	0.27	0/1564	0.54	0/2123
3	AB	0.29	0/1564	0.55	0/2123
4	B	0.23	0/3886	0.34	1/5293 (0.0%)
4	BE	0.24	0/3886	0.36	1/5293 (0.0%)
4	b	0.22	0/3886	0.35	0/5293
4	v	0.23	0/3886	0.32	0/5293
5	2	0.35	0/2816	0.40	1/3837 (0.0%)
5	BG	0.32	1/2816 (0.0%)	0.41	0/3837
5	D	0.25	0/2816	0.35	0/3837
5	d	0.31	1/2816 (0.0%)	0.41	1/3837 (0.0%)
6	3	0.15	0/562	0.34	0/763
6	BH	0.17	0/562	0.33	0/763
6	E	0.15	0/562	0.34	0/763
6	e	0.15	0/562	0.30	0/763
7	4	0.17	0/230	0.34	0/311
7	BI	0.15	0/230	0.31	0/311
7	F	0.15	0/230	0.31	0/311
7	f	0.17	0/230	0.33	0/311
8	A2	0.29	0/1580	0.40	0/2146
8	Au	0.23	0/1607	0.33	0/2184
8	BB	0.31	0/1669	0.37	0/2270
8	BJ	0.15	0/1607	0.38	0/2184
8	BQ	0.19	0/1580	0.40	0/2146
8	Ba	0.19	0/1669	0.37	1/2270 (0.0%)
8	G	0.25	0/1607	0.38	1/2184 (0.0%)
8	N	0.28	0/1580	0.40	0/2146

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	Y	0.31	0/1669	0.39	1/2270 (0.0%)
8	g	0.15	0/1607	0.38	0/2184
8	n	0.26	0/1580	0.48	2/2146 (0.1%)
8	y	0.25	0/1669	0.46	1/2270 (0.0%)
9	Av	0.29	0/447	0.52	0/608
9	BK	0.27	0/447	0.48	0/608
9	H	0.28	0/447	0.48	1/608 (0.2%)
9	h	0.28	0/447	0.52	1/608 (0.2%)
10	Aw	0.28	0/294	0.41	0/397
10	BL	0.27	0/294	0.39	0/397
10	I	0.27	0/294	0.40	0/397
10	i	0.27	0/294	0.50	0/397
11	Ay	0.22	0/313	0.44	0/428
11	BN	0.22	0/313	0.45	0/428
11	K	0.20	0/313	0.40	0/428
11	k	0.21	0/313	0.45	0/428
12	Az	0.28	0/301	0.33	0/409
12	BO	0.25	0/301	0.30	0/409
12	L	0.25	0/301	0.39	0/409
12	l	0.26	0/301	0.33	0/409
13	A1	0.26	0/254	0.50	0/347
13	BP	0.27	0/254	0.53	0/347
13	M	0.31	0/254	0.53	0/347
13	m	0.26	0/254	0.53	0/347
14	A6	0.22	0/1715	0.37	0/2328
14	BV	0.17	0/1715	0.36	0/2328
14	S	0.19	0/1715	0.35	0/2328
14	s	0.16	0/1715	0.34	0/2328
15	A7	0.26	0/246	0.34	0/333
15	BW	0.29	0/246	0.36	0/333
15	T	0.33	0/246	0.43	0/333
15	t	0.21	0/246	0.33	0/333
16	A8	0.17	0/197	0.26	0/261
16	BX	0.15	0/197	0.36	0/261
16	U	0.16	0/197	0.28	0/261
16	u	0.16	0/197	0.34	0/261
17	A0	0.26	0/439	0.41	0/594
17	BY	0.21	0/439	0.33	0/594
17	W	0.26	0/439	0.43	1/594 (0.2%)
17	w	0.26	0/439	0.44	0/594
18	BA	0.15	0/250	0.42	0/339
18	BZ	0.16	0/250	0.39	0/339
18	X	0.15	0/250	0.42	0/339

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	x	0.16	0/250	0.44	0/339
19	BC	0.20	0/475	0.43	0/649
19	Bb	0.19	0/475	0.39	0/649
19	Z	0.23	0/475	0.49	0/649
19	z	0.19	0/475	0.37	0/649
20	A	0.27	0/2602	0.37	0/3546
20	BD	0.26	0/2602	0.37	0/3546
20	R	0.32	0/2602	0.42	1/3546 (0.0%)
20	a	0.25	0/2602	0.38	1/3546 (0.0%)
21	1	0.28	0/3487	0.37	0/4750
21	BF	0.27	0/3478	0.35	0/4736
21	C	0.24	0/3487	0.36	0/4750
21	c	0.26	0/3478	0.38	0/4736
22	BU	0.35	0/1585	0.48	0/2161
22	r	0.31	0/1585	0.52	0/2161
All	All	0.26	2/109588 (0.0%)	0.40	20/149064 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	6	0	1
3	8	0	1
5	2	0	1
17	w	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	d	346	VAL	CB-CG1	-5.66	1.33	1.52
5	BG	346	VAL	CB-CG1	-5.54	1.34	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	167	MET	CG-SD-CE	-9.25	80.54	100.90
8	y	89	PRO	CA-N-CD	-8.75	99.75	112.00
20	a	328	MET	CG-SD-CE	-7.01	85.48	100.90
8	n	226	MET	CG-SD-CE	-6.92	85.69	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	167	MET	CG-SD-CE	-6.76	86.02	100.90
8	G	169	MET	CG-SD-CE	-6.54	86.52	100.90
4	BE	25	MET	CG-SD-CE	-6.31	87.02	100.90
8	n	223	MET	CG-SD-CE	-5.97	87.76	100.90
2	0	91	LYS	CD-CE-NZ	-5.90	93.01	111.90
4	B	106	LEU	CB-CG-CD1	-5.89	93.02	110.70
8	Y	226	MET	CG-SD-CE	-5.57	88.65	100.90
2	6	209	LEU	CB-CG-CD2	-5.55	94.03	110.70
8	Ba	169	MET	CG-SD-CE	-5.38	89.06	100.90
9	H	43	MET	CG-SD-CE	-5.34	89.15	100.90
5	d	200	MET	N-CA-CB	-5.34	102.26	110.16
2	6	93	ARG	CD-NE-CZ	-5.25	117.05	124.40
9	h	43	MET	CG-SD-CE	-5.21	89.43	100.90
17	W	133	LEU	CB-CG-CD1	-5.20	95.11	110.70
20	R	304	GLN	CA-CB-CG	5.18	124.46	114.10
5	2	266	ARG	CB-CG-CD	-5.04	99.70	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2	266	ARG	Sidechain
2	6	93	ARG	Sidechain
3	8	223	ARG	Sidechain
17	w	84	ARG	Sidechain

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	5	1529	0	1470	72	0
1	7	1530	0	1473	68	0
1	9	1529	0	1470	68	0
1	AA	1530	0	1473	82	0
2	0	1716	0	1658	115	0
2	6	1716	0	1658	113	0
3	8	1512	0	1444	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AB	1512	0	1444	95	0
4	B	3757	0	3641	84	0
4	BE	3757	0	3641	88	0
4	b	3757	0	3641	93	0
4	v	3757	0	3641	83	0
5	2	2723	0	2615	68	0
5	BG	2723	0	2615	85	0
5	D	2723	0	2615	65	0
5	d	2723	0	2615	99	0
6	3	544	0	519	17	0
6	BH	544	0	519	20	0
6	E	544	0	519	18	0
6	e	544	0	519	21	0
7	4	225	0	233	10	0
7	BI	225	0	233	13	0
7	F	225	0	233	9	0
7	f	225	0	233	13	0
8	A2	1536	0	1480	44	0
8	Au	1562	0	1503	43	0
8	BB	1621	0	1550	36	0
8	BJ	1562	0	1503	47	0
8	BQ	1536	0	1480	49	0
8	Ba	1621	0	1550	35	0
8	G	1562	0	1503	52	0
8	N	1536	0	1480	42	0
8	Y	1621	0	1550	43	0
8	g	1562	0	1503	47	0
8	n	1536	0	1480	51	0
8	y	1621	0	1550	42	0
9	Av	438	0	465	27	0
9	BK	438	0	465	23	0
9	H	438	0	465	19	0
9	h	438	0	465	29	0
10	Aw	286	0	295	2	0
10	BL	286	0	295	7	0
10	I	286	0	295	7	0
10	i	286	0	295	10	0
11	Ay	302	0	313	5	0
11	BN	302	0	313	4	0
11	K	302	0	313	5	0
11	k	302	0	313	9	0
12	Az	293	0	283	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BO	293	0	283	12	0
12	L	293	0	283	13	0
12	l	293	0	283	16	0
13	A1	250	0	279	16	0
13	BP	250	0	279	15	0
13	M	250	0	279	15	0
13	m	250	0	279	15	0
14	A6	1670	0	1649	36	0
14	BV	1670	0	1649	74	0
14	S	1670	0	1649	42	0
14	s	1670	0	1649	67	0
15	A7	239	0	255	9	0
15	BW	239	0	255	5	0
15	T	239	0	255	12	0
15	t	239	0	255	8	0
16	A8	195	0	206	14	0
16	BX	195	0	206	8	0
16	U	195	0	206	16	0
16	u	195	0	206	11	0
17	A0	428	0	405	13	0
17	BY	428	0	405	4	0
17	W	428	0	405	17	0
17	w	428	0	405	8	0
18	BA	248	0	266	7	0
18	BZ	248	0	266	8	0
18	X	248	0	266	8	0
18	x	248	0	266	7	0
19	BC	465	0	495	16	0
19	Bb	465	0	495	15	0
19	Z	465	0	495	16	0
19	z	465	0	495	17	0
20	A	2525	0	2443	50	0
20	BD	2525	0	2443	68	0
20	R	2525	0	2443	58	0
20	a	2525	0	2443	65	0
21	1	3373	0	3302	58	0
21	BF	3365	0	3295	62	0
21	C	3373	0	3302	60	0
21	c	3365	0	3295	81	0
22	BU	1539	0	1502	75	0
22	r	1539	0	1502	93	0
23	0	314	0	238	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	5	307	0	228	43	0
23	6	314	0	238	42	0
23	7	304	0	222	32	0
23	8	184	0	124	10	0
23	9	307	0	228	40	0
23	A2	358	0	318	47	0
23	A6	195	0	136	15	0
23	AA	304	0	222	34	0
23	AB	184	0	124	15	0
23	Au	349	0	300	39	0
23	BB	358	0	318	48	0
23	BH	45	0	28	0	0
23	BJ	351	0	303	54	0
23	BQ	358	0	318	51	0
23	BU	222	0	179	36	0
23	BV	195	0	136	20	0
23	Ba	358	0	318	45	0
23	G	349	0	300	50	0
23	N	358	0	318	45	0
23	S	195	0	136	15	0
23	Y	358	0	318	47	0
23	e	45	0	28	0	0
23	g	351	0	303	52	0
23	n	358	0	318	54	0
23	r	222	0	179	35	0
23	s	195	0	136	20	0
23	y	358	0	318	45	0
24	0	426	0	373	37	0
24	1	780	0	864	34	0
24	2	130	0	144	8	0
24	5	412	0	348	41	0
24	6	426	0	373	43	0
24	7	389	0	311	28	0
24	8	266	0	194	20	0
24	9	412	0	348	37	0
24	A	240	0	242	14	0
24	A2	473	0	468	23	0
24	A6	463	0	390	14	0
24	AA	389	0	311	28	0
24	AB	266	0	194	25	0
24	Au	477	0	477	20	0
24	Aw	65	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	1040	0	1152	73	0
24	BB	473	0	468	18	0
24	BD	240	0	242	18	0
24	BE	1040	0	1152	69	0
24	BF	845	0	936	39	0
24	BG	130	0	144	8	0
24	BJ	477	0	477	25	0
24	BQ	473	0	468	27	0
24	BU	518	0	452	36	0
24	BV	465	0	393	29	0
24	Ba	473	0	468	21	0
24	C	780	0	864	36	0
24	D	130	0	144	7	0
24	G	477	0	477	21	0
24	I	65	0	72	3	0
24	N	473	0	468	23	0
24	R	240	0	242	12	0
24	S	463	0	390	20	0
24	Y	473	0	468	22	0
24	a	240	0	242	17	0
24	b	1040	0	1152	74	0
24	c	845	0	936	47	0
24	d	130	0	144	7	0
24	g	477	0	477	21	0
24	n	473	0	468	25	0
24	r	518	0	452	37	0
24	s	465	0	393	29	0
24	v	1040	0	1152	79	0
24	y	473	0	468	19	0
25	0	84	0	112	19	0
25	5	84	0	112	15	0
25	6	84	0	112	17	0
25	7	84	0	112	13	0
25	8	42	0	56	6	0
25	9	84	0	112	18	0
25	A2	84	0	112	12	0
25	A6	84	0	112	10	0
25	AA	84	0	112	14	0
25	AB	42	0	56	9	0
25	Au	84	0	112	12	0
25	BB	84	0	112	11	0
25	BJ	84	0	112	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BQ	84	0	112	11	0
25	BU	42	0	56	10	0
25	BV	84	0	112	10	0
25	Ba	84	0	112	7	0
25	G	84	0	112	11	0
25	N	84	0	112	10	0
25	S	84	0	112	11	0
25	Y	84	0	112	9	0
25	g	84	0	112	16	0
25	n	84	0	112	11	0
25	r	42	0	56	9	0
25	s	84	0	112	16	0
25	y	84	0	112	9	0
26	5	44	0	56	1	0
26	7	44	0	56	5	0
26	9	44	0	56	1	0
26	A2	44	0	56	3	0
26	A6	44	0	56	2	0
26	AA	44	0	56	4	0
26	Au	44	0	56	1	0
26	BB	88	0	112	8	0
26	BJ	44	0	56	1	0
26	BQ	44	0	56	3	0
26	BV	44	0	56	5	0
26	Ba	44	0	56	2	0
26	G	44	0	56	1	0
26	N	44	0	56	3	0
26	S	44	0	56	3	0
26	Y	44	0	56	1	0
26	g	44	0	56	1	0
26	n	44	0	56	3	0
26	r	44	0	56	5	0
26	s	44	0	56	5	0
26	y	44	0	56	3	0
27	0	47	0	67	8	0
27	1	98	0	148	4	0
27	2	95	0	139	1	0
27	5	41	0	55	3	0
27	6	47	0	67	5	0
27	9	41	0	55	3	0
27	A0	49	0	74	1	0
27	A2	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Au	49	0	74	4	0
27	Az	49	0	74	3	0
27	B	95	0	139	2	0
27	BB	49	0	74	7	0
27	BE	144	0	213	3	0
27	BF	98	0	148	3	0
27	BG	49	0	74	1	0
27	BJ	49	0	74	4	0
27	BQ	49	0	74	6	0
27	BU	42	0	57	5	0
27	BY	49	0	74	1	0
27	Ba	49	0	74	4	0
27	C	98	0	148	5	0
27	D	49	0	74	3	0
27	G	49	0	74	3	0
27	L	49	0	74	3	0
27	N	49	0	74	5	0
27	W	49	0	74	1	0
27	Y	49	0	74	6	0
27	b	144	0	213	6	0
27	c	98	0	148	3	0
27	d	49	0	74	1	0
27	g	49	0	74	4	0
27	n	49	0	74	5	0
27	r	42	0	57	6	0
27	v	49	0	74	2	0
27	w	49	0	74	1	0
27	y	49	0	74	5	0
28	5	44	0	56	11	0
28	7	88	0	112	4	0
28	8	44	0	56	6	0
28	9	44	0	56	11	0
28	A2	44	0	56	6	0
28	AA	88	0	112	6	0
28	AB	44	0	56	6	0
28	Au	44	0	56	4	0
28	BB	44	0	56	6	0
28	BJ	44	0	56	1	0
28	BQ	44	0	56	5	0
28	BU	44	0	56	4	0
28	Ba	44	0	56	2	0
28	G	44	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	N	44	0	56	5	0
28	Y	44	0	56	5	0
28	g	44	0	56	1	0
28	n	44	0	56	2	0
28	r	44	0	56	5	0
28	y	44	0	56	3	0
29	1	80	0	112	7	0
29	4	40	0	56	3	0
29	8	40	0	56	6	0
29	A	40	0	56	3	0
29	AB	40	0	56	5	0
29	Av	40	0	56	4	0
29	Ay	80	0	112	8	0
29	B	160	0	224	20	0
29	BD	40	0	56	2	0
29	BE	160	0	224	15	0
29	BF	80	0	112	6	0
29	BI	40	0	56	2	0
29	BK	40	0	56	8	0
29	BN	40	0	56	2	0
29	Bb	40	0	56	3	0
29	C	80	0	112	5	0
29	F	40	0	56	1	0
29	H	40	0	56	5	0
29	K	80	0	112	5	0
29	R	40	0	56	1	0
29	a	40	0	56	3	0
29	b	160	0	224	16	0
29	c	40	0	56	3	0
29	f	40	0	56	2	0
29	h	40	0	56	7	0
29	k	40	0	56	1	0
29	v	160	0	224	16	0
29	z	80	0	112	8	0
30	1	102	0	144	5	0
30	2	46	0	62	0	0
30	A	48	0	66	1	0
30	A0	48	0	66	1	0
30	Aw	40	0	50	1	0
30	B	91	0	122	0	0
30	BE	51	0	72	1	0
30	BF	102	0	144	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	BG	46	0	62	0	0
30	BL	48	0	66	2	0
30	C	102	0	144	5	0
30	D	46	0	62	0	0
30	I	40	0	50	3	0
30	b	51	0	72	1	0
30	c	102	0	144	7	0
30	d	46	0	62	0	0
30	i	48	0	66	2	0
30	v	91	0	122	0	0
31	2	55	0	80	1	0
31	BG	55	0	80	2	0
31	D	55	0	80	1	0
31	d	55	0	80	3	0
32	2	50	0	67	3	0
32	A	54	0	78	8	0
32	A1	54	0	78	2	0
32	Az	42	0	48	3	0
32	BD	54	0	78	6	0
32	BG	50	0	67	4	0
32	BO	96	0	126	6	0
32	D	50	0	67	1	0
32	L	96	0	126	5	0
32	R	54	0	78	9	0
32	a	54	0	78	6	0
32	d	50	0	67	3	0
32	l	96	0	126	7	0
33	4	43	0	30	3	0
33	BI	43	0	30	2	0
33	F	43	0	30	1	0
33	f	43	0	30	2	0
34	1	177	0	228	7	0
34	A	59	0	76	2	0
34	Av	62	0	82	6	0
34	BD	119	0	154	2	0
34	BF	117	0	150	4	0
34	BK	62	0	82	6	0
34	C	177	0	228	5	0
34	H	62	0	82	6	0
34	R	59	0	76	2	0
34	a	119	0	154	3	0
34	c	117	0	150	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	h	62	0	82	4	0
35	2	4	0	1	0	0
35	A	4	0	1	0	0
35	BD	4	0	1	0	0
35	a	4	0	1	0	0
36	A	10	0	0	0	0
36	BD	10	0	0	1	0
36	R	10	0	0	0	0
36	a	10	0	0	1	0
37	A	1	0	0	0	0
37	BD	1	0	0	0	0
37	R	1	0	0	0	0
37	a	1	0	0	0	0
38	A	128	0	148	8	0
38	BD	128	0	148	6	0
38	R	128	0	148	7	0
38	a	128	0	148	4	0
All	All	146846	0	146920	4896	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 17.

All (4896) 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)
8:n:103:SER:HA	8:n:223:MET:HE1	1.25	1.18
8:BJ:226:MET:HE1	25:BJ:616:LUT:H12	1.27	1.14
4:BE:223:GLN:HE22	9:BK:35:PRO:HA	0.97	1.11
5:d:326:ILE:HG12	20:a:328:MET:HE1	1.39	1.05
2:0:172:GLY:HA3	1:AA:62:PHE:CE1	1.96	1.01
3:8:224:LEU:HD13	24:8:308:CLA:HMA3	1.43	1.00
2:6:149:ASN:HB3	19:Bb:1:MET:HE2	1.40	0.98
8:A2:107:MET:HE1	24:A2:610:CLA:HAB	1.46	0.96
4:BE:223:GLN:NE2	9:BK:35:PRO:HA	1.80	0.96
2:6:108:PHE:CE2	24:6:604:CLA:HAC1	2.00	0.96
23:5:609:CHL:HHC	23:6:601:CHL:H52	1.46	0.94
4:b:223:GLN:HE22	9:h:35:PRO:HA	1.31	0.94
5:D:266:ARG:HH12	20:A:220:THR:HG23	1.32	0.93
23:5:607:CHL:C10	23:5:607:CHL:C7	2.47	0.93
23:9:609:CHL:HHC	23:0:601:CHL:H52	1.48	0.93
24:5:610:CLA:H2	25:5:615:LUT:H26	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G:608:CHL:C10	23:G:608:CHL:C7	2.47	0.92
23:9:607:CHL:C7	23:9:607:CHL:C10	2.47	0.92
23:y:310:CHL:C10	23:y:310:CHL:C7	2.48	0.92
23:AA:308:CHL:C7	23:AA:308:CHL:C10	2.47	0.92
23:Au:609:CHL:C10	23:Au:609:CHL:C7	2.48	0.92
23:S:606:CHL:C7	23:S:606:CHL:C10	2.48	0.92
23:N:609:CHL:C7	23:N:609:CHL:C10	2.48	0.92
23:0:601:CHL:C10	23:0:601:CHL:C7	2.48	0.92
23:BQ:609:CHL:C7	23:BQ:609:CHL:C10	2.48	0.92
23:BU:607:CHL:C9	23:BU:607:CHL:C7	2.48	0.92
23:y:302:CHL:C9	23:y:302:CHL:C7	2.48	0.92
23:BJ:608:CHL:C10	23:BJ:608:CHL:C7	2.48	0.92
23:BQ:608:CHL:C7	23:BQ:608:CHL:C10	2.48	0.91
23:n:608:CHL:C7	23:n:608:CHL:C10	2.49	0.91
23:BV:606:CHL:C7	23:BV:606:CHL:C10	2.48	0.91
23:6:601:CHL:C10	23:6:601:CHL:C9	2.49	0.91
23:A6:606:CHL:C7	23:A6:606:CHL:C10	2.48	0.91
23:G:609:CHL:C7	23:G:609:CHL:C10	2.47	0.91
23:g:608:CHL:C7	23:g:608:CHL:C10	2.48	0.91
23:Au:608:CHL:C10	23:Au:608:CHL:C7	2.47	0.91
23:s:606:CHL:C7	23:s:606:CHL:C10	2.48	0.91
23:7:308:CHL:C7	23:7:308:CHL:C10	2.49	0.91
23:r:607:CHL:C10	23:r:607:CHL:C7	2.49	0.91
24:9:610:CLA:H2	25:9:615:LUT:H26	1.50	0.91
23:Ba:310:CHL:C10	23:Ba:310:CHL:C7	2.48	0.91
23:7:310:CHL:C7	23:7:310:CHL:C10	2.50	0.91
23:Y:309:CHL:C7	23:Y:309:CHL:C10	2.49	0.91
5:d:230:ALA:HA	21:c:457:LYS:NZ	1.86	0.91
23:n:609:CHL:C7	23:n:609:CHL:C10	2.48	0.91
8:Au:226:MET:HG2	25:Au:616:LUT:H12	1.52	0.91
23:A2:609:CHL:C10	23:A2:609:CHL:C7	2.48	0.91
23:BB:302:CHL:C7	23:BB:302:CHL:C9	2.49	0.91
2:6:108:PHE:HE2	24:6:604:CLA:HAC1	1.32	0.90
23:N:601:CHL:C9	23:N:601:CHL:C7	2.49	0.90
23:r:607:CHL:C7	23:r:607:CHL:C9	2.48	0.90
23:A2:609:CHL:C10	23:A2:609:CHL:C9	2.48	0.90
23:Au:601:CHL:C9	23:Au:601:CHL:C7	2.48	0.90
23:N:609:CHL:C10	23:N:609:CHL:C9	2.50	0.90
23:g:609:CHL:C7	23:g:609:CHL:C10	2.49	0.90
23:r:605:CHL:C10	23:r:605:CHL:C7	2.49	0.90
23:AA:310:CHL:C10	23:AA:310:CHL:C7	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:615:LUT:H171	25:S:615:LUT:H8	1.53	0.90
23:9:609:CHL:C7	23:9:609:CHL:C10	2.49	0.90
23:G:601:CHL:C7	23:G:601:CHL:C9	2.49	0.90
23:0:601:CHL:C10	23:0:601:CHL:C9	2.48	0.90
23:A6:606:CHL:C7	23:A6:606:CHL:C9	2.50	0.90
23:BJ:609:CHL:C10	23:BJ:609:CHL:C7	2.49	0.90
23:G:609:CHL:C7	23:G:609:CHL:C9	2.50	0.90
23:Y:308:CHL:C10	23:Y:308:CHL:C9	2.50	0.90
23:g:609:CHL:C7	23:g:609:CHL:C9	2.50	0.90
23:y:309:CHL:C10	23:y:309:CHL:C7	2.49	0.90
23:G:607:CHL:C10	23:G:607:CHL:C9	2.50	0.90
23:BJ:609:CHL:C7	23:BJ:609:CHL:C9	2.50	0.90
23:0:609:CHL:C7	23:0:609:CHL:C9	2.50	0.90
23:Au:609:CHL:C7	23:Au:609:CHL:C9	2.50	0.90
23:BU:607:CHL:C7	23:BU:607:CHL:C10	2.49	0.90
23:5:609:CHL:C10	23:5:609:CHL:C7	2.49	0.90
23:7:308:CHL:C7	23:7:308:CHL:C9	2.50	0.90
23:BQ:609:CHL:C7	23:BQ:609:CHL:C9	2.50	0.90
23:Ba:309:CHL:C10	23:Ba:309:CHL:C7	2.49	0.90
23:7:310:CHL:C7	23:7:310:CHL:C9	2.49	0.89
23:N:607:CHL:C9	23:N:607:CHL:C10	2.51	0.89
23:S:606:CHL:C7	23:S:606:CHL:C9	2.50	0.89
23:Y:302:CHL:C9	23:Y:302:CHL:C7	2.49	0.89
23:0:609:CHL:C7	23:0:609:CHL:C10	2.50	0.89
23:6:609:CHL:C7	23:6:609:CHL:C10	2.50	0.89
23:N:608:CHL:C10	23:N:608:CHL:C9	2.51	0.89
23:Y:310:CHL:C10	23:Y:310:CHL:C7	2.50	0.89
23:A2:601:CHL:C9	23:A2:601:CHL:C7	2.49	0.89
23:A2:607:CHL:C10	23:A2:607:CHL:C7	2.51	0.89
23:BB:302:CHL:C7	23:BB:302:CHL:C10	2.50	0.89
23:BB:310:CHL:C9	23:BB:310:CHL:C7	2.50	0.89
23:BU:605:CHL:C10	23:BU:605:CHL:C7	2.49	0.89
23:AA:310:CHL:C7	23:AA:310:CHL:C9	2.50	0.89
23:BQ:601:CHL:C10	23:BQ:601:CHL:C7	2.50	0.89
23:7:308:CHL:C10	23:7:308:CHL:C9	2.51	0.89
23:Au:607:CHL:C10	23:Au:607:CHL:C9	2.50	0.89
23:6:609:CHL:C7	23:6:609:CHL:C9	2.50	0.89
23:N:608:CHL:C10	23:N:608:CHL:C7	2.49	0.89
23:9:609:CHL:C10	23:9:609:CHL:C9	2.51	0.89
23:A2:601:CHL:C7	23:A2:601:CHL:C10	2.51	0.89
23:y:310:CHL:C7	23:y:310:CHL:C9	2.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:309:CHL:C10	23:BB:309:CHL:C7	2.50	0.89
23:BB:310:CHL:C7	23:BB:310:CHL:C10	2.50	0.89
23:Ba:308:CHL:C10	23:Ba:308:CHL:C7	2.51	0.89
23:5:607:CHL:C7	23:5:607:CHL:C9	2.51	0.89
23:6:601:CHL:C10	23:6:601:CHL:C7	2.49	0.89
23:Y:310:CHL:C7	23:Y:310:CHL:C9	2.50	0.89
23:n:601:CHL:C10	23:n:601:CHL:C7	2.50	0.89
23:n:607:CHL:C7	23:n:607:CHL:C9	2.51	0.89
23:AA:308:CHL:C7	23:AA:308:CHL:C9	2.50	0.89
25:A6:615:LUT:H171	25:A6:615:LUT:H8	1.52	0.89
23:Ba:309:CHL:C7	23:Ba:309:CHL:C9	2.51	0.89
23:N:607:CHL:C9	23:N:607:CHL:C7	2.51	0.89
23:A2:608:CHL:C10	23:A2:608:CHL:C7	2.49	0.89
23:Ba:308:CHL:C7	23:Ba:308:CHL:C9	2.51	0.89
23:N:607:CHL:C10	23:N:607:CHL:C7	2.51	0.89
23:Y:308:CHL:C10	23:Y:308:CHL:C7	2.51	0.89
23:Y:309:CHL:C7	23:Y:309:CHL:C9	2.51	0.89
23:A2:608:CHL:C7	23:A2:608:CHL:C9	2.51	0.89
23:BB:308:CHL:C10	23:BB:308:CHL:C9	2.50	0.89
23:G:608:CHL:C7	23:G:608:CHL:C9	2.51	0.89
23:g:607:CHL:C10	23:g:607:CHL:C9	2.51	0.89
23:g:608:CHL:C7	23:g:608:CHL:C9	2.51	0.89
23:9:607:CHL:C7	23:9:607:CHL:C9	2.51	0.89
23:A2:607:CHL:C7	23:A2:607:CHL:C9	2.51	0.89
23:A2:608:CHL:C10	23:A2:608:CHL:C9	2.51	0.89
23:BJ:608:CHL:C7	23:BJ:608:CHL:C9	2.51	0.89
23:g:607:CHL:C9	23:g:607:CHL:C7	2.51	0.88
23:n:607:CHL:C7	23:n:607:CHL:C10	2.50	0.88
23:n:609:CHL:C7	23:n:609:CHL:C9	2.50	0.88
23:s:606:CHL:C7	23:s:606:CHL:C9	2.51	0.88
23:BQ:601:CHL:C7	23:BQ:601:CHL:C9	2.51	0.88
23:BQ:607:CHL:C7	23:BQ:607:CHL:C10	2.50	0.88
23:BV:606:CHL:C7	23:BV:606:CHL:C9	2.51	0.88
23:Ba:302:CHL:C9	23:Ba:302:CHL:C7	2.51	0.88
23:BU:605:CHL:C7	23:BU:605:CHL:C9	2.51	0.88
23:5:607:CHL:C10	23:5:607:CHL:C9	2.51	0.88
23:5:609:CHL:C10	23:5:609:CHL:C9	2.51	0.88
23:N:601:CHL:C7	23:N:601:CHL:C10	2.51	0.88
23:N:609:CHL:C7	23:N:609:CHL:C9	2.51	0.88
23:g:601:CHL:C7	23:g:601:CHL:C10	2.50	0.88
23:Au:608:CHL:C7	23:Au:608:CHL:C9	2.51	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A2:607:CHL:C10	23:A2:607:CHL:C9	2.50	0.88
23:BB:309:CHL:C10	23:BB:309:CHL:C9	2.52	0.88
23:BB:309:CHL:C7	23:BB:309:CHL:C9	2.51	0.88
23:9:607:CHL:C10	23:9:607:CHL:C9	2.50	0.88
23:Au:608:CHL:C10	23:Au:608:CHL:C9	2.52	0.88
23:y:308:CHL:C7	23:y:308:CHL:C10	2.51	0.88
23:y:309:CHL:C7	23:y:309:CHL:C9	2.51	0.88
23:r:606:CHL:C10	23:r:606:CHL:C9	2.52	0.88
23:BB:310:CHL:C9	23:BB:310:CHL:C10	2.51	0.88
23:BJ:607:CHL:C10	23:BJ:607:CHL:C9	2.51	0.88
23:Ba:302:CHL:C7	23:Ba:302:CHL:C10	2.50	0.88
23:Y:309:CHL:C10	23:Y:309:CHL:C9	2.51	0.88
23:BJ:608:CHL:C10	23:BJ:608:CHL:C9	2.51	0.88
23:BQ:607:CHL:C7	23:BQ:607:CHL:C9	2.51	0.88
23:Ba:310:CHL:C7	23:Ba:310:CHL:C9	2.51	0.88
23:g:601:CHL:C7	23:g:601:CHL:C9	2.51	0.88
23:s:606:CHL:C10	23:s:606:CHL:C9	2.52	0.88
23:r:605:CHL:C7	23:r:605:CHL:C9	2.51	0.88
23:A2:609:CHL:C7	23:A2:609:CHL:C9	2.51	0.88
23:BU:606:CHL:C10	23:BU:606:CHL:C9	2.52	0.88
23:G:607:CHL:C9	23:G:607:CHL:C7	2.52	0.88
23:n:607:CHL:C9	23:n:607:CHL:C10	2.51	0.88
24:s:610:CLA:HAA1	24:s:610:CLA:HED2	1.56	0.88
21:c:78:GLU:HB2	21:c:79:LYS:HZ2	1.38	0.88
23:BB:308:CHL:C10	23:BB:308:CHL:C7	2.51	0.88
23:BJ:601:CHL:C7	23:BJ:601:CHL:C10	2.51	0.88
23:Ba:308:CHL:C10	23:Ba:308:CHL:C9	2.52	0.88
23:Y:302:CHL:C7	23:Y:302:CHL:C10	2.50	0.88
23:y:308:CHL:C7	23:y:308:CHL:C9	2.51	0.88
23:y:309:CHL:C10	23:y:309:CHL:C9	2.52	0.88
23:r:606:CHL:C10	23:r:606:CHL:C7	2.51	0.88
24:v:607:CLA:H18	5:2:282:MET:HE1	1.54	0.88
23:Au:607:CHL:C9	23:Au:607:CHL:C7	2.52	0.88
23:Au:609:CHL:C10	23:Au:609:CHL:C9	2.52	0.88
23:BU:606:CHL:C9	23:BU:606:CHL:C7	2.52	0.88
2:0:224:MET:HG2	25:0:616:LUT:H12	1.56	0.88
23:Au:601:CHL:C7	23:Au:601:CHL:C10	2.52	0.88
23:BV:606:CHL:C10	23:BV:606:CHL:C9	2.52	0.88
23:N:608:CHL:C9	23:N:608:CHL:C7	2.51	0.87
23:n:601:CHL:C7	23:n:601:CHL:C9	2.51	0.87
23:n:608:CHL:C10	23:n:608:CHL:C9	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BJ:601:CHL:C7	23:BJ:601:CHL:C9	2.51	0.87
23:BJ:607:CHL:C10	23:BJ:607:CHL:C7	2.52	0.87
23:BJ:607:CHL:C9	23:BJ:607:CHL:C7	2.51	0.87
23:BQ:607:CHL:C10	23:BQ:607:CHL:C9	2.51	0.87
23:Ba:309:CHL:C10	23:Ba:309:CHL:C9	2.52	0.87
23:g:608:CHL:C10	23:g:608:CHL:C9	2.51	0.87
23:Au:601:CHL:C9	23:Au:601:CHL:C10	2.51	0.87
23:y:302:CHL:C7	23:y:302:CHL:C10	2.52	0.87
23:AA:308:CHL:C10	23:AA:308:CHL:C9	2.52	0.87
23:G:607:CHL:C10	23:G:607:CHL:C7	2.52	0.87
23:n:609:CHL:C10	23:n:609:CHL:C9	2.53	0.87
23:s:605:CHL:HBB1	25:s:615:LUT:H161	1.56	0.87
23:BU:606:CHL:C10	23:BU:606:CHL:C7	2.51	0.87
23:n:608:CHL:C7	23:n:608:CHL:C9	2.53	0.87
23:BB:302:CHL:C9	23:BB:302:CHL:C10	2.52	0.87
11:BN:40:MET:HE1	29:BN:101:BCR:HC41	1.57	0.87
23:G:608:CHL:C10	23:G:608:CHL:C9	2.52	0.87
23:g:607:CHL:C10	23:g:607:CHL:C7	2.53	0.87
23:y:302:CHL:C9	23:y:302:CHL:C10	2.53	0.87
23:r:606:CHL:C9	23:r:606:CHL:C7	2.52	0.87
23:9:609:CHL:C7	23:9:609:CHL:C9	2.53	0.87
23:Au:607:CHL:C10	23:Au:607:CHL:C7	2.52	0.87
23:BU:607:CHL:C9	23:BU:607:CHL:C10	2.53	0.87
23:Y:302:CHL:C9	23:Y:302:CHL:C10	2.53	0.87
23:Y:308:CHL:C9	23:Y:308:CHL:C7	2.52	0.87
23:Y:310:CHL:C10	23:Y:310:CHL:C9	2.51	0.87
23:y:308:CHL:C10	23:y:308:CHL:C9	2.52	0.87
23:BQ:608:CHL:C10	23:BQ:608:CHL:C9	2.52	0.87
20:R:184:ILE:HG23	20:R:328:MET:HE3	1.54	0.87
2:6:224:MET:HG2	25:6:616:LUT:H12	1.56	0.87
8:G:226:MET:HG2	25:G:616:LUT:H12	1.56	0.87
23:G:609:CHL:C10	23:G:609:CHL:C9	2.53	0.87
23:BQ:609:CHL:C10	23:BQ:609:CHL:C9	2.53	0.87
23:G:601:CHL:C7	23:G:601:CHL:C10	2.52	0.87
23:n:601:CHL:C10	23:n:601:CHL:C9	2.53	0.87
23:y:310:CHL:C10	23:y:310:CHL:C9	2.53	0.87
21:c:71:GLU:HG2	21:c:89:LEU:HD13	1.57	0.87
23:BV:605:CHL:HBB1	25:BV:615:LUT:H161	1.57	0.87
23:G:601:CHL:C9	23:G:601:CHL:C10	2.52	0.86
23:r:607:CHL:C10	23:r:607:CHL:C9	2.53	0.86
23:A6:606:CHL:C10	23:A6:606:CHL:C9	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A2:601:CHL:C9	23:A2:601:CHL:C10	2.52	0.86
17:w:84:ARG:HH12	20:a:97:TRP:C	1.82	0.86
24:BV:610:CLA:HAA1	24:BV:610:CLA:HED2	1.58	0.86
23:Ba:310:CHL:C10	23:Ba:310:CHL:C9	2.53	0.86
23:BQ:601:CHL:C10	23:BQ:601:CHL:C9	2.53	0.86
23:BQ:608:CHL:C7	23:BQ:608:CHL:C9	2.53	0.86
23:5:609:CHL:C7	23:5:609:CHL:C9	2.53	0.86
23:BB:308:CHL:C9	23:BB:308:CHL:C7	2.52	0.86
8:G:214:LYS:HE2	24:G:611:CLA:O2D	1.76	0.86
23:N:601:CHL:C9	23:N:601:CHL:C10	2.53	0.86
23:S:606:CHL:C10	23:S:606:CHL:C9	2.53	0.86
22:r:250:MET:HE1	24:r:602:CLA:HHC	1.57	0.86
23:6:601:CHL:C9	23:6:601:CHL:C7	2.52	0.86
23:0:601:CHL:C7	23:0:601:CHL:C9	2.53	0.86
23:BJ:601:CHL:C10	23:BJ:601:CHL:C9	2.54	0.86
14:BV:69:ILE:HG22	14:BV:71:LEU:H	1.40	0.86
8:BQ:102:HIS:HB3	8:BQ:223:MET:HE1	1.57	0.85
23:g:609:CHL:C10	23:g:609:CHL:C9	2.54	0.85
23:BU:605:CHL:C10	23:BU:605:CHL:C9	2.54	0.85
23:Ba:302:CHL:C9	23:Ba:302:CHL:C10	2.55	0.85
22:BU:168:ALA:O	22:BU:172:GLU:HG2	1.77	0.85
14:s:100:LEU:HD11	24:s:602:CLA:H11	1.57	0.85
23:g:601:CHL:C10	23:g:601:CHL:C9	2.55	0.85
23:AA:310:CHL:C10	23:AA:310:CHL:C9	2.55	0.85
23:7:310:CHL:C10	23:7:310:CHL:C9	2.55	0.84
8:g:226:MET:HE1	25:g:616:LUT:H12	1.58	0.84
23:BJ:609:CHL:C10	23:BJ:609:CHL:C9	2.54	0.84
23:r:605:CHL:C10	23:r:605:CHL:C9	2.54	0.84
1:5:226:MET:SD	25:5:616:LUT:H12	2.17	0.83
3:8:194:TYR:HE2	3:8:225:LYS:HG2	1.42	0.83
28:7:301:XAT:H41	23:7:308:CHL:HBA2	1.60	0.83
4:BE:223:GLN:HE22	9:BK:35:PRO:CA	1.86	0.83
5:D:200:MET:HE2	5:D:282:MET:HG2	1.57	0.83
22:r:168:ALA:O	22:r:172:GLU:HG2	1.76	0.83
8:g:226:MET:HE1	25:g:616:LUT:H10	1.60	0.83
14:S:162:TYR:HB2	14:S:167:ILE:HD11	1.61	0.83
23:6:609:CHL:C10	23:6:609:CHL:C9	2.56	0.83
22:BU:250:MET:HE1	24:BU:602:CLA:HHC	1.61	0.83
5:d:265:LYS:HE2	20:a:245:THR:HG22	1.60	0.83
9:Av:40:THR:HA	9:Av:43:MET:HG2	1.61	0.82
23:BQ:607:CHL:HBB2	23:BQ:609:CHL:HBC1	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:609:CHL:C9	23:0:609:CHL:C10	2.56	0.82
8:BJ:226:MET:CE	25:BJ:616:LUT:H12	2.08	0.82
11:k:40:MET:HE1	29:k:101:BCR:HC41	1.60	0.82
21:c:78:GLU:HB2	21:c:79:LYS:NZ	1.92	0.82
4:b:223:GLN:NE2	9:h:35:PRO:HA	1.94	0.82
20:A:196:PRO:HA	20:A:199:MET:HE3	1.62	0.82
23:n:607:CHL:HBB2	23:n:609:CHL:HBC1	1.62	0.82
23:BJ:607:CHL:HBB2	23:BJ:609:CHL:HBC1	1.62	0.82
3:8:256:LEU:HD21	25:8:311:LUT:H172	1.61	0.81
3:AB:256:LEU:HD21	25:AB:311:LUT:H172	1.62	0.81
4:B:224:ARG:HH22	9:H:37:TRP:HA	1.45	0.81
28:N:619:XAT:H28	27:Y:319:LHG:H372	1.63	0.81
1:9:223:MET:HE1	24:9:602:CLA:HHC	1.63	0.81
28:A2:619:XAT:H28	27:BB:319:LHG:H372	1.62	0.81
8:n:103:SER:HA	8:n:223:MET:CE	2.09	0.81
4:BE:41:GLU:HB3	4:BE:60:MET:HE1	1.61	0.81
2:0:224:MET:HE2	2:0:224:MET:HA	1.63	0.81
14:S:122:MET:HE1	24:S:609:CLA:HAB	1.62	0.80
2:0:91:LYS:NZ	1:AA:82:THR:O	2.14	0.80
5:BG:163:LEU:HD23	34:BK:102:DGD:HBE1	1.62	0.80
28:AA:301:XAT:H41	23:AA:308:CHL:HBA2	1.61	0.80
23:g:607:CHL:HBB2	23:g:609:CHL:HBC1	1.61	0.80
2:0:167:MET:HE1	23:0:609:CHL:CHC	2.11	0.80
23:BJ:609:CHL:C9	23:BJ:609:CHL:H112	2.12	0.80
2:6:224:MET:HE2	2:6:224:MET:HA	1.64	0.80
26:A2:617:NEX:H192	26:A2:617:NEX:H183	1.63	0.80
23:g:609:CHL:C9	23:g:609:CHL:H112	2.11	0.80
20:R:196:PRO:HA	20:R:199:MET:HE3	1.63	0.80
4:v:224:ARG:HH22	9:Av:37:TRP:HA	1.45	0.79
11:K:40:MET:HE1	29:K:101:BCR:H332	1.62	0.79
6:e:30:LEU:HD21	7:f:22:VAL:HG13	1.64	0.79
14:BV:123:LEU:HG	24:BV:604:CLA:HAB	1.65	0.79
5:d:323:ASN:HA	5:d:326:ILE:HD12	1.62	0.79
2:6:167:MET:HE1	23:6:609:CHL:CHC	2.13	0.79
4:v:472:ARG:HH22	24:v:611:CLA:CGD	1.95	0.79
14:S:188:TYR:HE1	14:S:194:LEU:HG	1.48	0.78
21:c:71:GLU:HG3	21:c:86:LEU:HD22	1.64	0.78
23:AA:310:CHL:C9	23:AA:310:CHL:H112	2.14	0.78
1:5:223:MET:HE1	24:5:602:CLA:HHC	1.65	0.78
29:B:623:BCR:HC31	32:a:412:SQD:H222	1.65	0.78
4:b:472:ARG:HG3	4:b:479:PHE:CE2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:230:ALA:HA	21:BF:457:LYS:NZ	1.98	0.78
23:y:307:CHL:HMC	23:y:308:CHL:C4C	2.13	0.78
8:A2:231:VAL:HG21	24:A2:613:CLA:HAC2	1.66	0.78
24:a:407:CLA:HED2	24:a:407:CLA:H2A	1.65	0.78
1:AA:226:MET:HG2	25:AA:317:LUT:H12	1.66	0.78
23:Au:609:CHL:C9	23:Au:609:CHL:H112	2.14	0.78
8:N:231:VAL:HG21	24:N:613:CLA:HAC2	1.65	0.78
5:2:266:ARG:HE	5:2:266:ARG:C	1.91	0.78
10:I:2:LEU:HD13	17:W:85:MET:HE2	1.64	0.78
24:BJ:612:CLA:HHC	24:BJ:612:CLA:HBB1	1.66	0.78
22:BU:258:VAL:HG11	24:BU:612:CLA:HAC2	1.66	0.78
24:7:303:CLA:H2	25:7:317:LUT:H26	1.66	0.77
3:8:110:MET:SD	3:8:232:SER:HA	2.24	0.77
23:G:609:CHL:C9	23:G:609:CHL:H112	2.15	0.77
8:g:220:ARG:HA	8:g:223:MET:HE3	1.66	0.77
14:A6:122:MET:HE1	24:A6:609:CLA:HAB	1.63	0.77
5:BG:200:MET:HE1	5:BG:282:MET:HE2	1.65	0.77
23:Ba:307:CHL:HMC	23:Ba:308:CHL:C4C	2.13	0.77
24:y:311:CLA:H92	24:y:311:CLA:H41	1.67	0.77
1:5:217:LYS:NZ	27:5:618:LHG:O4	2.18	0.77
4:b:226:TYR:CD2	4:b:231:MET:HB2	2.20	0.77
5:2:257:ILE:HG12	20:R:133:LEU:HD23	1.66	0.77
2:0:234:THR:HG23	2:0:236:LYS:H	1.49	0.77
23:BU:605:CHL:C9	23:BU:605:CHL:H112	2.15	0.77
23:r:605:CHL:C9	23:r:605:CHL:H112	2.15	0.77
23:7:310:CHL:C9	23:7:310:CHL:H112	2.14	0.77
24:B:606:CLA:HBB1	24:B:606:CLA:HHC	1.66	0.77
2:0:236:LYS:HB3	2:0:240:GLU:OE2	1.85	0.77
24:g:612:CLA:HBB1	24:g:612:CLA:HHC	1.66	0.77
24:n:614:CLA:HHC	24:n:614:CLA:HBB1	1.66	0.77
4:B:472:ARG:HH22	24:B:611:CLA:CGD	1.97	0.77
11:Ay:40:MET:HE1	29:Ay:101:BCR:HC41	1.65	0.77
24:BQ:614:CLA:HHC	24:BQ:614:CLA:HBB1	1.66	0.77
22:r:59:TYR:HE2	24:r:601:CLA:H3A	1.50	0.76
23:G:607:CHL:HBB2	23:G:609:CHL:HBC1	1.65	0.76
4:B:282:GLN:HG2	16:U:100:ILE:HD13	1.68	0.76
4:b:282:GLN:HG2	16:u:100:ILE:HD13	1.67	0.76
22:r:258:VAL:HG11	24:r:612:CLA:HAC2	1.66	0.76
24:8:310:CLA:HBA2	24:8:310:CLA:HBD	1.68	0.76
13:A1:11:THR:O	13:A1:15:ILE:HG13	1.86	0.76
8:BQ:168:LEU:HD11	26:BQ:617:NEX:H34	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:101:SER:OG	20:A:103:ASP:OD2	2.04	0.76
21:c:165:LEU:HD21	24:c:507:CLA:HAB	1.66	0.76
2:6:90:ALA:O	2:6:93:ARG:HG2	1.86	0.76
4:v:282:GLN:HG2	16:A8:100:ILE:HD13	1.67	0.76
1:5:108:LEU:HD22	24:5:604:CLA:HAB	1.67	0.76
1:9:217:LYS:NZ	27:9:618:LHG:O4	2.17	0.76
24:AB:310:CLA:HBD	24:AB:310:CLA:HBA2	1.68	0.76
24:b:607:CLA:HHC	24:b:607:CLA:HBB1	1.67	0.75
29:v:622:BCR:HC31	32:BD:412:SQD:H222	1.66	0.75
10:Aw:2:LEU:HD13	17:A0:85:MET:HE2	1.68	0.75
2:6:167:MET:HA	2:6:170:VAL:HG12	1.67	0.75
23:BB:309:CHL:HBB1	23:BB:309:CHL:HHC	1.68	0.75
22:BU:189:SER:HA	22:BU:192:ILE:HD12	1.69	0.75
8:n:106:ALA:HB2	8:n:223:MET:SD	2.27	0.75
24:v:606:CLA:HHC	24:v:606:CLA:HBB1	1.66	0.75
8:Au:111:LEU:HD11	24:Au:612:CLA:HAB	1.67	0.75
4:BE:384:ARG:NH1	5:BG:350:GLY:O	2.19	0.75
5:d:200:MET:HE2	5:d:282:MET:HE2	1.68	0.75
23:6:601:CHL:HHC	23:6:601:CHL:HBB1	1.68	0.75
4:b:223:GLN:HE22	9:h:35:PRO:CA	2.00	0.75
11:Ay:36:ILE:HD11	11:Ay:40:MET:HE2	1.68	0.75
24:BE:607:CLA:HBB1	24:BE:607:CLA:HHC	1.68	0.75
28:BQ:619:XAT:H28	27:Ba:319:LHG:H372	1.69	0.75
2:6:221:MET:HE1	24:6:602:CLA:HAB	1.67	0.75
23:6:609:CHL:C9	23:6:609:CHL:H112	2.17	0.75
5:D:283:SER:OG	24:D:401:CLA:O1D	2.05	0.75
17:W:133:LEU:H	17:W:133:LEU:HD12	1.50	0.75
23:Y:309:CHL:HHC	23:Y:309:CHL:HBB1	1.67	0.75
23:0:609:CHL:C9	23:0:609:CHL:H112	2.17	0.75
8:BQ:231:VAL:HG11	24:BQ:613:CLA:HAC2	1.68	0.75
8:n:166:VAL:HG23	23:n:609:CHL:HBB2	1.69	0.74
1:9:162:TRP:O	1:9:166:VAL:HG23	1.87	0.74
23:6:606:CHL:HBB2	23:6:607:CHL:HBB1	1.67	0.74
21:c:26:ARG:HH12	24:c:512:CLA:HBD	1.52	0.74
1:AA:231:VAL:HG11	24:AA:314:CLA:HAC2	1.68	0.74
32:A1:101:SQD:H122	29:BE:618:BCR:H383	1.67	0.74
24:BD:407:CLA:H2A	24:BD:407:CLA:HED2	1.68	0.74
23:5:606:CHL:HMC	25:5:616:LUT:H163	1.68	0.74
5:D:137:VAL:HG23	5:D:139:LEU:HD23	1.70	0.74
4:BE:60:MET:HE2	4:BE:63:ILE:HD12	1.68	0.74
20:R:45:THR:O	20:R:49:ILE:HD12	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:103:SER:HB2	8:N:219:GLY:HA3	1.69	0.74
8:g:106:ALA:HB3	8:g:223:MET:HG2	1.70	0.74
8:G:107:MET:HE1	24:G:610:CLA:HAB	1.70	0.74
4:b:384:ARG:NH1	5:d:350:GLY:O	2.20	0.74
8:n:231:VAL:HG11	24:n:613:CLA:HAC2	1.68	0.74
2:0:167:MET:HA	2:0:170:VAL:HG12	1.68	0.74
23:A6:601:CHL:HHC	23:A6:601:CHL:HBB1	1.68	0.74
32:L:103:SQD:H122	29:b:618:BCR:H383	1.68	0.74
23:S:601:CHL:HBB1	23:S:601:CHL:HHC	1.69	0.74
23:0:601:CHL:HBB1	23:0:601:CHL:HHC	1.69	0.74
4:v:472:ARG:HH12	24:v:611:CLA:HED3	1.53	0.74
21:c:76:VAL:HG12	21:c:79:LYS:HZ3	1.52	0.74
23:Au:601:CHL:C9	23:Au:601:CHL:H112	2.18	0.74
23:BJ:601:CHL:C9	23:BJ:601:CHL:H112	2.18	0.74
1:7:231:VAL:HG11	24:7:314:CLA:HAC2	1.69	0.74
23:BB:302:CHL:C9	23:BB:302:CHL:H112	2.18	0.74
8:BQ:166:VAL:HG23	23:BQ:609:CHL:HBB2	1.70	0.74
21:BF:165:LEU:HD21	24:BF:507:CLA:HAB	1.70	0.73
5:D:187:GLN:HB2	24:D:401:CLA:HBC1	1.71	0.73
21:c:81:MET:HE3	21:c:90:PRO:HG3	1.70	0.73
2:0:52:ARG:O	2:0:54:LYS:NZ	2.20	0.73
6:3:71:ASP:N	16:A8:103:TYR:OH	2.17	0.73
28:n:619:XAT:H28	27:y:319:LHG:H372	1.69	0.73
8:Au:107:MET:HE1	24:Au:610:CLA:HAB	1.68	0.73
23:g:601:CHL:C9	23:g:601:CHL:H112	2.19	0.73
2:0:197:LEU:H	2:0:197:LEU:HD12	1.53	0.73
4:B:226:TYR:HA	4:B:231:MET:HE3	1.71	0.73
2:0:240:GLU:HA	2:0:243:LEU:HG	1.68	0.73
5:2:193:THR:HG23	24:2:402:CLA:HBC2	1.70	0.73
6:E:71:ASP:N	16:U:103:TYR:OH	2.17	0.73
5:d:150:PRO:HA	5:d:153:VAL:HG12	1.70	0.73
23:G:601:CHL:C9	23:G:601:CHL:H112	2.19	0.73
23:Au:601:CHL:H51	23:BB:310:CHL:HBB1	1.68	0.73
2:6:221:MET:HE1	24:6:602:CLA:HHC	1.69	0.73
5:2:232:THR:OG1	20:R:269:ARG:NH1	2.21	0.73
21:BF:48:LYS:HE2	21:BF:138:GLU:HG3	1.71	0.73
22:r:159:TRP:HD1	22:r:160:LEU:HD22	1.53	0.72
8:BB:226:MET:HG2	25:BB:317:LUT:H12	1.71	0.72
14:BV:123:LEU:HG	24:BV:604:CLA:CAB	2.19	0.72
5:BG:187:GLN:HB2	24:BG:401:CLA:HBC1	1.70	0.72
5:D:193:THR:HG23	24:D:401:CLA:HBC2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:79:GLY:HA3	3:8:229:ILE:HD13	1.71	0.72
9:H:40:THR:HA	9:H:43:MET:HG2	1.72	0.72
14:s:123:LEU:HG	24:s:604:CLA:HAB	1.71	0.72
5:2:187:GLN:HB2	24:2:402:CLA:HBC1	1.70	0.72
2:6:242:LEU:HD21	25:6:615:LUT:H21	1.72	0.72
24:B:614:CLA:HED2	24:B:614:CLA:H2A	1.72	0.72
24:v:604:CLA:H92	24:v:604:CLA:H41	1.70	0.72
21:BF:81:MET:HG2	21:BF:86:LEU:HD12	1.70	0.72
2:6:52:ARG:O	2:6:54:LYS:NZ	2.20	0.72
1:5:107:MET:CE	24:5:610:CLA:HHC	2.19	0.72
4:b:55:MET:HE1	4:b:64:PRO:HB3	1.72	0.72
23:AA:302:CHL:HBB1	23:AA:302:CHL:HHC	1.72	0.72
4:BE:55:MET:HE1	4:BE:64:PRO:HB3	1.72	0.72
21:1:165:LEU:HD21	24:1:506:CLA:HAB	1.72	0.72
23:G:601:CHL:H51	23:Y:310:CHL:HBB1	1.71	0.71
13:A1:24:ILE:HD13	13:BP:24:ILE:HD13	1.72	0.71
2:6:104:MET:HE1	24:6:610:CLA:HAB	1.70	0.71
24:n:610:CLA:H62	24:n:612:CLA:HBA1	1.71	0.71
5:BG:193:THR:HG23	24:BG:401:CLA:HBC2	1.73	0.71
8:y:89:PRO:HD2	8:y:90:GLU:H	1.54	0.71
4:b:223:GLN:NE2	9:h:34:ALA:O	2.24	0.71
24:BQ:610:CLA:H62	24:BQ:612:CLA:HBA1	1.70	0.71
3:8:105:HIS:HD1	28:8:312:XAT:H15	1.55	0.71
24:B:604:CLA:H41	24:B:604:CLA:H92	1.70	0.71
8:Y:226:MET:HG2	25:Y:317:LUT:H12	1.73	0.71
23:Y:302:CHL:C9	23:Y:302:CHL:H112	2.19	0.71
14:s:221:LEU:HB3	24:s:609:CLA:HMA2	1.73	0.71
23:7:302:CHL:HHC	23:7:302:CHL:HBB1	1.73	0.71
4:B:187:VAL:HG11	9:H:67:LEU:HD11	1.73	0.71
23:G:609:CHL:HHC	23:N:601:CHL:H52	1.72	0.71
14:A6:149:LYS:HA	23:A6:606:CHL:HED1	1.72	0.71
5:BG:219:VAL:HG11	20:BD:272:HIS:CD2	2.25	0.71
1:9:114:VAL:HG23	1:9:241:LEU:HD11	1.73	0.71
24:B:609:CLA:CAD	9:H:43:MET:HE1	2.20	0.71
24:Y:311:CLA:H41	24:Y:311:CLA:H92	1.72	0.71
23:0:606:CHL:HBB2	23:0:607:CHL:HBB1	1.72	0.71
24:v:614:CLA:HED2	24:v:614:CLA:H2A	1.73	0.71
4:BE:282:GLN:HG2	16:BX:100:ILE:HD13	1.73	0.71
23:9:606:CHL:HMC	25:9:616:LUT:H163	1.72	0.70
21:BF:269:GLU:HG2	21:BF:448:ALA:HB2	1.72	0.70
20:A:188:ALA:HB2	20:A:328:MET:HE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:229:GLY:O	14:S:233:MET:HG3	1.92	0.70
4:v:187:VAL:HG11	9:Av:67:LEU:HD11	1.73	0.70
8:A2:103:SER:HB2	8:A2:219:GLY:HA3	1.72	0.70
19:Z:57:LEU:HD22	19:Z:60:LEU:HD21	1.72	0.70
12:L:13:LEU:HD21	13:M:26:TYR:HA	1.74	0.70
8:g:226:MET:CE	25:g:616:LUT:H12	2.22	0.70
23:BQ:609:CHL:HHC	23:BQ:609:CHL:HBB1	1.72	0.70
5:D:257:ILE:HG12	20:A:133:LEU:HD23	1.73	0.70
24:s:610:CLA:HAB	27:c:520:LHG:H101	1.73	0.70
21:c:362:ARG:HD2	21:c:370:ARG:HH12	1.56	0.70
8:Y:252:VAL:HG23	8:Y:253:ASN:OD1	1.91	0.70
8:g:210:GLU:O	8:g:214:LYS:HG2	1.91	0.70
14:s:102:LYS:HD2	2:0:179:ASP:HB3	1.72	0.70
21:C:381:LYS:HG3	21:C:382:LYS:HG3	1.74	0.70
5:2:137:VAL:HG23	5:2:139:LEU:HD23	1.72	0.70
23:A2:607:CHL:HHC	23:A2:607:CHL:HBB1	1.74	0.70
1:5:107:MET:HE1	24:5:610:CLA:HHC	1.73	0.70
1:7:168:LEU:HD12	26:7:319:NEX:H34	1.74	0.70
4:B:472:ARG:HH12	24:B:611:CLA:HED3	1.54	0.70
2:0:104:MET:HE1	24:0:610:CLA:HAB	1.73	0.70
1:5:158:ILE:O	1:5:161:ILE:HG22	1.92	0.70
1:5:108:LEU:HD22	24:5:604:CLA:CAB	2.22	0.70
13:M:24:ILE:HD13	13:m:24:ILE:HD13	1.72	0.70
14:S:149:LYS:HA	23:S:606:CHL:HED1	1.73	0.70
1:9:226:MET:SD	25:9:616:LUT:H12	2.31	0.70
23:5:609:CHL:C9	23:5:609:CHL:H112	2.22	0.69
23:N:601:CHL:C9	23:N:601:CHL:H112	2.22	0.69
8:BJ:210:GLU:O	8:BJ:214:LYS:HG2	1.91	0.69
4:b:317:ASN:HA	4:b:330:MET:HE1	1.74	0.69
20:A:288:LEU:HD12	21:C:432:VAL:HG22	1.74	0.69
5:d:219:VAL:HG11	20:a:272:HIS:CD2	2.27	0.69
24:A2:614:CLA:HHC	24:A2:614:CLA:HBB1	1.74	0.69
26:BB:320:NEX:H181	26:BB:320:NEX:H193	1.73	0.69
20:R:153:ALA:HB1	24:R:404:CLA:HED1	1.75	0.69
24:BB:311:CLA:H92	24:BB:311:CLA:H41	1.74	0.69
4:b:226:TYR:HA	4:b:231:MET:HG3	1.74	0.69
3:AB:127:TRP:CD1	3:AB:127:TRP:H	2.11	0.69
24:BE:605:CLA:H92	24:BE:605:CLA:H41	1.73	0.69
1:9:108:LEU:HD22	24:9:604:CLA:HAB	1.74	0.69
1:AA:230:PHE:CE2	1:AA:234:ILE:HG13	2.27	0.69
3:AB:79:GLY:HA3	3:AB:229:ILE:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:114:VAL:HG23	1:5:241:LEU:HD11	1.74	0.69
1:7:160:ALA:O	1:7:164:THR:HG23	1.92	0.69
5:d:233:PHE:HA	20:a:269:ARG:HD3	1.73	0.69
5:d:257:ILE:HG12	20:a:133:LEU:HD23	1.75	0.69
21:C:165:LEU:HD21	24:C:506:CLA:HAB	1.74	0.69
22:r:199:ILE:HA	22:r:202:ILE:HG22	1.74	0.69
22:r:214:LYS:HD3	22:r:218:PRO:HA	1.75	0.69
26:r:617:NEX:H181	26:r:617:NEX:H193	1.74	0.69
2:0:206:PHE:O	2:0:210:LYS:HG3	1.93	0.69
23:A2:601:CHL:C9	23:A2:601:CHL:H112	2.22	0.69
23:N:606:CHL:HBB1	25:N:616:LUT:H161	1.75	0.69
4:BE:317:ASN:HA	4:BE:330:MET:HE1	1.75	0.69
34:R:401:DGD:HBH1	32:R:411:SQD:H341	1.75	0.69
3:8:127:TRP:CD1	3:8:127:TRP:H	2.11	0.69
3:8:223:ARG:HD2	3:8:224:LEU:N	2.08	0.69
23:N:607:CHL:HHC	23:N:607:CHL:HBB1	1.75	0.69
8:Y:211:LEU:HA	8:Y:214:LYS:HG2	1.75	0.69
21:C:342:MET:SD	21:C:352:GLY:HA2	2.33	0.69
1:9:108:LEU:HD22	24:9:604:CLA:CAB	2.23	0.69
23:A2:606:CHL:HBB1	25:A2:616:LUT:H161	1.75	0.69
6:BH:58:GLU:N	6:BH:58:GLU:OE2	2.24	0.69
21:BF:362:ARG:HD2	21:BF:370:ARG:HH12	1.57	0.69
24:N:614:CLA:HHC	24:N:614:CLA:HBB1	1.74	0.68
2:0:91:LYS:HZ3	1:AA:83:ALA:C	2.01	0.68
1:AA:55:ARG:O	1:AA:57:LYS:NZ	2.21	0.68
5:BG:283:SER:OG	24:BG:401:CLA:O1D	2.10	0.68
23:BQ:608:CHL:H152	26:BQ:617:NEX:H402	1.75	0.68
8:G:103:SER:HB2	8:G:219:GLY:HA3	1.76	0.68
24:b:605:CLA:H41	24:b:605:CLA:H92	1.74	0.68
21:C:418:ASN:HB2	34:C:518:DGD:HE2	1.76	0.68
23:9:609:CHL:C9	23:9:609:CHL:H112	2.23	0.68
24:0:613:CLA:H12	24:0:614:CLA:CAD	2.23	0.68
3:AB:120:GLN:NE2	3:AB:125:VAL:O	2.26	0.68
12:Az:8:GLU:HG3	32:Az:101:SQD:H62	1.75	0.68
14:A6:202:PRO:HB3	23:A6:607:CHL:HBC3	1.76	0.68
8:BB:211:LEU:HA	8:BB:214:LYS:HG2	1.74	0.68
24:BV:610:CLA:HAB	27:BF:521:LHG:H101	1.74	0.68
14:s:118:ALA:HB1	14:s:229:GLY:HA3	1.75	0.68
5:BG:160:ILE:HD12	5:BG:288:VAL:HG22	1.74	0.68
3:8:110:MET:HE1	3:8:231:HIS:HB3	1.75	0.68
3:8:160:ARG:NH2	23:8:307:CHL:O1D	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AA:303:CLA:H2	25:AA:317:LUT:H26	1.76	0.68
3:8:223:ARG:NH1	3:8:224:LEU:HB3	2.08	0.68
12:Az:13:LEU:HD21	13:A1:26:TYR:HA	1.74	0.68
23:BV:601:CHL:HBB1	23:BV:601:CHL:HHC	1.76	0.68
3:AB:105:HIS:HD1	28:AB:312:XAT:H15	1.59	0.68
8:BQ:103:SER:O	8:BQ:107:MET:HG2	1.94	0.68
21:1:418:ASN:HB2	34:1:518:DGD:HE2	1.76	0.68
2:6:206:PHE:O	2:6:210:LYS:HG3	1.94	0.68
8:G:231:VAL:HG11	24:G:613:CLA:HAC2	1.76	0.68
23:G:609:CHL:C9	23:G:609:CHL:C11	2.72	0.68
20:A:45:THR:O	20:A:49:ILE:HG13	1.93	0.68
23:Au:609:CHL:C9	23:Au:609:CHL:C11	2.72	0.68
24:BE:609:CLA:CAB	5:BG:124:ILE:HD13	2.24	0.68
2:0:144:TYR:HD1	2:0:145:LEU:HG	1.59	0.68
9:H:49:LEU:HB3	29:H:101:BCR:H14C	1.75	0.67
20:A:153:ALA:HB1	24:A:405:CLA:HED1	1.75	0.67
23:r:605:CHL:C9	23:r:605:CHL:C11	2.73	0.67
23:9:601:CHL:HED3	24:9:602:CLA:HBC2	1.76	0.67
23:BJ:609:CHL:C9	23:BJ:609:CHL:C11	2.72	0.67
1:5:138:ILE:CD1	1:5:158:ILE:HB	2.24	0.67
23:s:601:CHL:HHC	23:s:601:CHL:HBB1	1.77	0.67
3:8:120:GLN:NE2	3:8:125:VAL:O	2.28	0.67
14:S:115:LEU:HD22	14:S:200:LEU:HD12	1.76	0.67
8:BJ:103:SER:HB2	8:BJ:219:GLY:HA3	1.76	0.67
8:G:91:THR:O	8:G:95:ASN:ND2	2.27	0.67
17:w:84:ARG:NH2	20:a:99:ALA:O	2.28	0.67
14:A6:115:LEU:HD22	14:A6:200:LEU:HD12	1.75	0.67
2:6:234:THR:HG21	2:6:241:ASN:HD21	1.60	0.67
2:6:144:TYR:HD1	2:6:145:LEU:HG	1.59	0.67
23:g:609:CHL:C9	23:g:609:CHL:C11	2.72	0.67
21:1:39:ASN:HB2	24:1:508:CLA:HBA1	1.77	0.67
19:z:1:MET:HE2	2:0:149:ASN:HB3	1.77	0.67
23:BU:606:CHL:C10	23:BU:606:CHL:H62	2.24	0.67
8:G:111:LEU:HD11	24:G:612:CLA:HAB	1.76	0.67
12:L:13:LEU:HD22	13:M:25:ILE:HG22	1.76	0.67
5:d:47:GLY:O	5:d:51:THR:HG23	1.95	0.67
6:e:58:GLU:N	6:e:58:GLU:OE2	2.28	0.67
22:r:212:SER:HA	22:r:215:ARG:HG3	1.76	0.67
1:AA:168:LEU:HD12	26:AA:319:NEX:H34	1.76	0.67
4:v:474:LEU:O	5:2:135:ARG:NH2	2.28	0.67
23:BB:302:CHL:C9	23:BB:302:CHL:C11	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BP:5:ILE:H	13:BP:5:ILE:HD12	1.60	0.67
5:d:43:TYR:OH	7:f:19:GLY:O	2.12	0.67
34:A:402:DGD:HBH1	32:A:413:SQD:H341	1.75	0.67
23:AA:310:CHL:C9	23:AA:310:CHL:C11	2.73	0.67
23:Y:302:CHL:C9	23:Y:302:CHL:C11	2.73	0.67
29:v:617:BCR:H383	32:BO:101:SQD:H122	1.77	0.67
5:BG:257:ILE:HG12	20:BD:133:LEU:HD23	1.76	0.67
22:BU:250:MET:HE1	24:BU:602:CLA:HAB	1.76	0.67
5:d:237:ASN:HB3	5:d:240:GLN:HB3	1.77	0.66
12:Az:13:LEU:HD22	13:A1:25:ILE:HG22	1.76	0.66
23:BU:605:CHL:C9	23:BU:605:CHL:C11	2.72	0.66
1:AA:158:ILE:HA	1:AA:161:ILE:HD12	1.76	0.66
23:5:607:CHL:HAA1	28:5:619:XAT:H41	1.76	0.66
10:i:6:LEU:O	10:i:10:THR:HG23	1.95	0.66
27:9:618:LHG:H132	28:AA:301:XAT:H403	1.78	0.66
28:BQ:619:XAT:H14	27:Ba:319:LHG:H191	1.78	0.66
1:5:226:MET:SD	25:5:616:LUT:H10	2.35	0.66
4:B:99:ALA:HB1	24:B:606:CLA:H61	1.77	0.66
5:d:200:MET:CE	5:d:282:MET:HE2	2.25	0.66
6:3:30:LEU:HD21	7:4:22:VAL:HG13	1.76	0.66
1:5:187:GLU:CD	1:5:187:GLU:H	2.04	0.66
4:B:474:LEU:O	5:D:135:ARG:NH2	2.28	0.66
22:BU:234:LYS:HA	22:BU:237:GLN:HE21	1.61	0.66
23:BU:605:CHL:HMC	23:BU:606:CHL:C1C	2.26	0.66
24:6:613:CLA:H12	24:6:614:CLA:CAD	2.24	0.66
3:8:222:GLU:HA	3:8:225:LYS:HD2	1.78	0.66
4:B:416:THR:HA	4:B:419:LYS:HE3	1.77	0.66
5:d:173:SER:HB3	5:d:178:ALA:HB1	1.78	0.66
21:c:269:GLU:HG2	21:c:448:ALA:HB2	1.77	0.66
23:Au:601:CHL:C9	23:Au:601:CHL:C11	2.74	0.66
8:BJ:169:MET:HA	8:BJ:172:VAL:HG22	1.78	0.66
1:5:107:MET:HE2	24:5:610:CLA:HMC3	1.77	0.66
2:6:90:ALA:HA	2:6:93:ARG:HD2	1.76	0.66
17:W:100:LEU:O	17:W:104:ILE:HG12	1.95	0.66
8:Au:133:LYS:O	8:Au:137:GLN:NE2	2.29	0.66
27:5:618:LHG:H132	28:7:301:XAT:H403	1.78	0.66
13:m:5:ILE:HD12	13:m:5:ILE:H	1.61	0.66
1:9:176:ARG:HH12	23:9:609:CHL:HED1	1.61	0.66
5:BG:237:ASN:HB3	5:BG:240:GLN:HB3	1.78	0.66
3:8:183:GLU:H	3:8:183:GLU:CD	2.03	0.66
8:Au:91:THR:O	8:Au:95:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Au:103:SER:HB2	8:Au:219:GLY:HA3	1.78	0.66
2:6:55:TYR:HB3	2:6:75:TYR:HB3	1.78	0.65
3:AB:153:MET:HE1	23:AB:307:CHL:C4C	2.25	0.65
5:BG:266:ARG:NH2	20:BD:245:THR:OG1	2.29	0.65
26:N:617:NEX:H192	26:N:617:NEX:H183	1.76	0.65
20:R:101:SER:OG	20:R:103:ASP:OD2	2.13	0.65
4:BE:99:ALA:HB1	24:BE:607:CLA:H61	1.78	0.65
23:BJ:601:CHL:C9	23:BJ:601:CHL:C11	2.74	0.65
4:b:99:ALA:HB1	24:b:607:CLA:H61	1.78	0.65
14:s:103:LYS:HD3	14:s:106:ASN:HD22	1.61	0.65
22:r:250:MET:HE1	24:r:602:CLA:HAB	1.78	0.65
23:r:606:CHL:C10	23:r:606:CHL:H62	2.26	0.65
4:v:99:ALA:HB1	24:v:606:CLA:H61	1.77	0.65
1:5:107:MET:HE1	24:5:610:CLA:CAB	2.26	0.65
1:7:108:LEU:HD13	24:7:305:CLA:HBB2	1.77	0.65
3:8:200:PHE:HB3	24:8:308:CLA:OBD	1.96	0.65
20:A:259:ILE:HG23	20:A:260:PHE:H	1.62	0.65
24:v:609:CLA:C3D	9:Av:43:MET:HE1	2.27	0.65
7:4:20:LEU:O	7:4:24:THR:OG1	2.15	0.65
20:R:259:ILE:HG23	20:R:260:PHE:H	1.61	0.65
20:R:288:LEU:HD12	21:1:432:VAL:HG22	1.76	0.65
21:1:142:GLU:N	21:1:142:GLU:OE2	2.30	0.65
21:1:269:GLU:HG2	21:1:448:ALA:HB2	1.78	0.65
21:c:142:GLU:N	21:c:142:GLU:OE1	2.29	0.65
22:r:144:GLY:HA3	22:r:246:ALA:HB1	1.78	0.65
4:v:224:ARG:NH2	9:Av:37:TRP:HA	2.10	0.65
24:Ba:311:CLA:H92	24:Ba:311:CLA:H41	1.78	0.65
4:B:14:ASN:ND2	12:L:7:ASN:OD1	2.27	0.65
29:B:617:BCR:H383	32:l:101:SQD:H122	1.77	0.65
23:n:601:CHL:C9	23:n:601:CHL:H112	2.27	0.65
5:2:266:ARG:NH2	5:2:266:ARG:O	2.27	0.65
23:A6:605:CHL:HMC	23:A6:606:CHL:C4C	2.27	0.65
14:BV:118:ALA:HB1	14:BV:229:GLY:HA3	1.78	0.65
23:7:310:CHL:C9	23:7:310:CHL:C11	2.74	0.65
3:8:148:THR:O	3:8:152:LEU:HD12	1.97	0.65
2:0:188:TYR:HE2	2:0:210:LYS:HE3	1.61	0.65
14:BV:172:VAL:O	14:BV:176:VAL:HG13	1.97	0.65
22:BU:169:GLY:HA2	22:BU:172:GLU:OE1	1.97	0.65
6:E:30:LEU:HD21	7:F:22:VAL:HG13	1.77	0.65
23:N:601:CHL:C9	23:N:601:CHL:C11	2.75	0.65
28:9:619:XAT:H203	24:0:613:CLA:H62	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ba:302:CHL:C9	23:Ba:302:CHL:H112	2.27	0.65
22:BU:144:GLY:HA3	22:BU:246:ALA:HB1	1.79	0.65
22:BU:172:GLU:OE2	23:BU:605:CHL:HAC1	1.97	0.65
4:B:224:ARG:NH2	9:H:37:TRP:HA	2.11	0.65
23:g:601:CHL:C9	23:g:601:CHL:C11	2.75	0.65
23:A2:601:CHL:C9	23:A2:601:CHL:C11	2.75	0.65
23:A2:606:CHL:HMC	23:A2:607:CHL:C4C	2.27	0.65
2:6:90:ALA:HA	2:6:93:ARG:CD	2.27	0.64
2:0:164:VAL:HG23	23:0:609:CHL:HBB2	1.78	0.64
1:AA:223:MET:HE1	24:AA:303:CLA:HMC3	1.79	0.64
8:BQ:107:MET:SD	8:BQ:219:GLY:HA2	2.37	0.64
1:7:223:MET:SD	1:7:224:PHE:N	2.70	0.64
4:B:462:PHE:HE1	24:B:611:CLA:HAB	1.62	0.64
8:n:111:LEU:HD11	8:n:115:PHE:CD1	2.31	0.64
8:n:180:ASN:ND2	8:n:185:GLU:OE1	2.29	0.64
2:0:165:ILE:O	2:0:169:LEU:HG	1.98	0.64
3:AB:183:GLU:CD	3:AB:183:GLU:H	2.03	0.64
26:BQ:617:NEX:H192	26:BQ:617:NEX:H183	1.79	0.64
3:8:222:GLU:O	3:8:226:LEU:HD22	1.98	0.64
23:N:608:CHL:HBA1	23:N:608:CHL:HBD	1.79	0.64
12:l:23:LEU:O	12:l:27:VAL:HG22	1.97	0.64
15:A7:2:GLU:OE1	15:A7:2:GLU:N	2.24	0.64
19:BC:49:GLY:O	19:BC:53:LEU:HG	1.97	0.64
8:BQ:180:ASN:ND2	8:BQ:185:GLU:OE1	2.29	0.64
2:6:149:ASN:HB3	19:Bb:1:MET:CE	2.21	0.64
3:8:194:TYR:CE2	3:8:225:LYS:HG2	2.31	0.64
6:E:30:LEU:HD23	7:F:25:VAL:HB	1.79	0.64
23:G:601:CHL:C9	23:G:601:CHL:C11	2.74	0.64
23:n:609:CHL:HHC	23:n:609:CHL:HBB1	1.79	0.64
1:AA:219:GLY:O	1:AA:223:MET:HG3	1.98	0.64
3:AB:148:THR:O	3:AB:152:LEU:HD12	1.98	0.64
8:BQ:172:VAL:HG11	23:BQ:608:CHL:HMA3	1.79	0.64
26:n:617:NEX:H192	26:n:617:NEX:H183	1.78	0.64
8:y:98:LEU:HD23	23:y:310:CHL:HED3	1.79	0.64
2:0:55:TYR:HB3	2:0:75:TYR:HB3	1.78	0.64
5:2:54:THR:HA	5:2:68:TYR:HD1	1.63	0.64
2:6:142:LEU:HD21	24:6:604:CLA:HAA2	1.80	0.64
23:6:609:CHL:C9	23:6:609:CHL:C11	2.75	0.64
8:g:169:MET:HA	8:g:172:VAL:HG22	1.77	0.64
21:C:130:ILE:HD12	21:C:134:LEU:HD23	1.79	0.64
8:Au:231:VAL:HG11	24:Au:613:CLA:HAC2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BV:221:LEU:HB3	24:BV:609:CLA:HMA2	1.80	0.64
5:d:232:THR:OG1	20:a:269:ARG:NH1	2.31	0.64
5:d:283:SER:OG	24:d:401:CLA:O1D	2.11	0.64
22:r:169:GLY:HA2	22:r:172:GLU:OE1	1.97	0.64
8:A2:128:GLU:OE1	8:A2:134:ALA:HA	1.97	0.64
21:1:58:GLY:O	21:1:122:SER:OG	2.16	0.64
1:5:103:SER:HB2	1:5:219:GLY:HA3	1.80	0.64
2:6:165:ILE:O	2:6:169:LEU:HG	1.98	0.64
8:N:69:TYR:OH	8:N:81:ASP:OD2	2.07	0.64
23:S:605:CHL:HMC	23:S:606:CHL:C4C	2.27	0.64
19:Z:49:GLY:O	19:Z:53:LEU:HG	1.97	0.64
1:AA:230:PHE:HE2	1:AA:234:ILE:HG13	1.63	0.64
4:v:14:ASN:ND2	12:Az:7:ASN:OD1	2.28	0.64
22:BU:134:GLN:OE1	22:BU:134:GLN:N	2.18	0.64
24:5:602:CLA:HAB	25:5:616:LUT:H32	1.79	0.64
4:b:462:PHE:HE1	24:b:612:CLA:HAB	1.63	0.64
8:y:103:SER:HB3	8:y:219:GLY:HA3	1.79	0.64
21:BF:82:TYR:HE1	21:BF:398:HIS:HD2	1.44	0.64
1:9:187:GLU:H	1:9:187:GLU:CD	2.06	0.64
23:0:609:CHL:C9	23:0:609:CHL:C11	2.75	0.64
5:BG:52:GLY:HA2	5:BG:56:VAL:HG12	1.80	0.64
5:BG:173:SER:HB3	5:BG:178:ALA:HB1	1.80	0.64
8:Ba:103:SER:HB3	8:Ba:219:GLY:HA3	1.79	0.64
23:5:601:CHL:HED3	24:5:602:CLA:HBC2	1.78	0.63
8:G:133:LYS:O	8:G:137:GLN:NE2	2.30	0.63
24:N:613:CLA:H91	27:N:618:LHG:H321	1.80	0.63
8:Y:107:MET:HE1	24:Y:311:CLA:HAB	1.79	0.63
20:a:131:TRP:HZ2	21:c:449:ARG:HD2	1.63	0.63
24:BU:602:CLA:H142	28:BU:616:XAT:H393	1.80	0.63
3:8:153:MET:HE1	23:8:307:CHL:C4C	2.28	0.63
11:K:40:MET:CE	29:K:101:BCR:H332	2.28	0.63
8:n:172:VAL:HG11	23:n:608:CHL:HMA3	1.79	0.63
7:F:20:LEU:O	7:F:24:THR:OG1	2.13	0.63
23:N:606:CHL:HMC	23:N:607:CHL:C4C	2.28	0.63
14:s:175:VAL:O	14:s:179:VAL:HG12	1.99	0.63
20:BD:331:MET:HE2	20:BD:331:MET:HA	1.80	0.63
8:n:92:PHE:O	8:n:96:ARG:HG3	1.98	0.63
15:t:6:TYR:O	15:t:10:LEU:HD13	1.98	0.63
24:A2:613:CLA:H91	27:A2:618:LHG:H321	1.80	0.63
22:r:172:GLU:OE2	23:r:605:CHL:HAC1	1.99	0.63
26:9:617:NEX:H192	26:9:617:NEX:H183	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:103:SER:HB2	8:g:219:GLY:HA3	1.79	0.63
21:C:39:ASN:HB2	24:C:508:CLA:HBA1	1.79	0.63
21:c:57:ALA:HA	21:c:60:ILE:HD12	1.81	0.63
4:v:121:GLU:O	9:Av:24:LYS:NZ	2.32	0.63
26:BB:318:NEX:H192	26:BB:318:NEX:H183	1.80	0.63
6:BH:69:ARG:HB2	16:BX:102:ARG:HH12	1.64	0.63
24:r:602:CLA:H142	28:r:616:XAT:H393	1.80	0.63
17:A0:124:GLU:OE1	17:A0:124:GLU:N	2.27	0.63
3:8:223:ARG:HH11	3:8:224:LEU:HB3	1.63	0.63
23:9:609:CHL:C9	23:9:609:CHL:C11	2.77	0.63
8:BB:149:ASN:HB3	8:BB:152:LEU:HD23	1.81	0.63
8:BQ:235:VAL:HG13	8:BQ:236:THR:HG23	1.81	0.63
38:BD:408:PHO:H41	32:BD:412:SQD:H223	1.81	0.63
2:6:188:TYR:HE2	2:6:210:LYS:HE3	1.64	0.63
21:C:58:GLY:O	21:C:122:SER:OG	2.16	0.63
1:AA:106:ALA:HB3	1:AA:223:MET:HB3	1.81	0.63
4:v:462:PHE:HE1	24:v:611:CLA:HAB	1.64	0.63
1:7:80:TRP:CD1	1:7:82:THR:HG23	2.34	0.62
5:D:79:VAL:HG22	5:D:174:PHE:HB2	1.81	0.62
5:d:180:PHE:O	5:d:183:ILE:HG22	1.99	0.62
23:BJ:609:CHL:HBB1	23:BJ:609:CHL:HHC	1.79	0.62
26:5:617:NEX:H192	26:5:617:NEX:H183	1.81	0.62
3:8:238:ALA:O	3:8:242:PHE:HD1	1.82	0.62
8:y:169:MET:HE1	23:y:310:CHL:C1C	2.30	0.62
20:A:131:TRP:HZ2	21:C:449:ARG:HD2	1.64	0.62
21:c:63:TRP:CZ2	21:c:67:MET:HG3	2.34	0.62
4:BE:250:PHE:HE2	24:BE:603:CLA:H193	1.63	0.62
5:d:200:MET:HE1	31:d:403:PL9:H272	1.82	0.62
8:n:235:VAL:HG13	8:n:236:THR:HG23	1.81	0.62
1:9:55:ARG:O	1:9:57:LYS:NZ	2.30	0.62
8:BQ:101:ILE:HD12	23:BQ:609:CHL:HED3	1.81	0.62
1:5:55:ARG:O	1:5:57:LYS:NZ	2.30	0.62
1:5:163:ALA:O	1:5:167:ILE:HG22	1.99	0.62
4:b:256:MET:SD	4:b:448:ARG:HG3	2.39	0.62
22:r:234:LYS:HA	22:r:237:GLN:HE21	1.64	0.62
23:BJ:601:CHL:H52	23:Ba:310:CHL:HHC	1.82	0.62
8:BQ:95:ASN:OD1	24:BQ:602:CLA:HHB	1.99	0.62
20:R:131:TRP:HZ2	21:1:449:ARG:HD2	1.64	0.62
23:6:607:CHL:HBB2	23:6:609:CHL:HBC1	1.82	0.62
8:Y:149:ASN:HB3	8:Y:152:LEU:HD23	1.81	0.62
5:d:230:ALA:HA	21:c:457:LYS:HZ1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g:609:CHL:HHC	23:g:609:CHL:HBB1	1.79	0.62
24:9:602:CLA:HAB	25:9:616:LUT:H32	1.80	0.62
23:5:609:CHL:C9	23:5:609:CHL:C11	2.76	0.62
8:N:165:GLN:HG3	23:N:606:CHL:HMA3	1.82	0.62
26:Y:318:NEX:H192	26:Y:318:NEX:H183	1.81	0.62
8:n:101:ILE:HD12	23:n:609:CHL:HED3	1.80	0.62
1:AA:128:GLU:O	1:AA:137:GLN:NE2	2.32	0.62
6:3:68:GLY:HA3	16:A8:103:TYR:HE1	1.65	0.62
8:N:226:MET:HG3	25:N:616:LUT:H12	1.81	0.62
1:AA:103:SER:O	1:AA:107:MET:HB2	1.99	0.62
3:AB:238:ALA:O	3:AB:242:PHE:HD1	1.83	0.62
29:AB:313:BCR:H371	29:AB:313:BCR:H403	1.81	0.62
23:A2:608:CHL:HBD	23:A2:608:CHL:HBA1	1.80	0.62
14:BV:149:LYS:HA	23:BV:606:CHL:HED1	1.82	0.62
1:7:128:GLU:O	1:7:137:GLN:NE2	2.33	0.62
8:N:128:GLU:OE1	8:N:134:ALA:HA	2.00	0.62
5:d:54:THR:HA	5:d:68:TYR:HD2	1.63	0.62
5:d:194:LEU:O	12:l:35:TYR:OH	2.17	0.62
14:s:149:LYS:HA	23:s:606:CHL:HED1	1.80	0.62
5:2:266:ARG:C	5:2:266:ARG:NE	2.58	0.62
6:3:30:LEU:HD23	7:4:25:VAL:HB	1.81	0.62
8:n:95:ASN:OD1	24:n:602:CLA:HHB	2.00	0.62
21:C:269:GLU:HG2	21:C:448:ALA:HB2	1.81	0.62
23:r:605:CHL:HMC	23:r:606:CHL:C1C	2.29	0.62
1:AA:105:TRP:O	1:AA:108:LEU:HD12	2.00	0.62
4:BE:256:MET:SD	4:BE:448:ARG:HG3	2.39	0.62
13:M:1:MET:HE3	13:M:2:GLU:N	2.14	0.62
23:n:606:CHL:HBB1	25:n:616:LUT:H161	1.81	0.62
5:2:283:SER:OG	24:2:402:CLA:O1D	2.15	0.62
4:BE:250:PHE:CE2	24:BE:603:CLA:H193	2.35	0.62
1:7:105:TRP:O	1:7:108:LEU:HD12	2.00	0.61
3:8:156:VAL:HG11	23:8:306:CHL:HMA3	1.81	0.61
34:a:401:DGD:HBH2	32:a:412:SQD:H341	1.82	0.61
38:a:408:PHO:H41	32:a:412:SQD:H223	1.82	0.61
23:9:607:CHL:HAA1	28:9:619:XAT:H41	1.82	0.61
8:Au:91:THR:HG22	8:Au:95:ASN:HD21	1.65	0.61
17:A0:133:LEU:HD23	17:A0:133:LEU:H	1.65	0.61
23:Ba:302:CHL:C9	23:Ba:302:CHL:C11	2.78	0.61
4:B:55:MET:HE1	4:B:267:LEU:HD22	1.82	0.61
5:D:54:THR:HA	5:D:68:TYR:HD1	1.64	0.61
21:C:267:SER:HB3	21:C:270:ALA:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:266:ARG:NH2	20:BD:226:GLU:OE1	2.33	0.61
20:R:88:ALA:HA	21:1:356:MET:CE	2.29	0.61
20:R:119:PHE:CE1	38:R:407:PHO:H142	2.35	0.61
6:E:68:GLY:HA3	16:U:103:TYR:HE1	1.65	0.61
17:w:84:ARG:NH1	20:a:97:TRP:O	2.33	0.61
20:a:332:HIS:NE2	36:a:403:OEX:O5	2.32	0.61
1:AA:163:ALA:O	1:AA:167:ILE:HG12	2.00	0.61
5:2:153:VAL:HG22	24:2:402:CLA:HED3	1.81	0.61
8:BJ:169:MET:HE1	23:BJ:609:CHL:C1C	2.31	0.61
4:B:384:ARG:HH11	20:A:334:ARG:HH21	1.48	0.61
6:E:74:GLU:OE1	6:E:74:GLU:N	2.33	0.61
21:C:181:TYR:N	21:C:198:LYS:HZ2	1.98	0.61
28:5:619:XAT:H241	23:6:601:CHL:C2C	2.31	0.61
28:5:619:XAT:H203	24:6:613:CLA:H102	1.81	0.61
24:s:602:CLA:H52	25:s:615:LUT:H28	1.83	0.61
18:x:94:GLY:HA2	18:x:97:LEU:HG	1.82	0.61
23:BB:307:CHL:HBB1	25:BB:317:LUT:H161	1.82	0.61
24:1:513:CLA:HBD	24:1:513:CLA:HBA1	1.81	0.61
2:6:100:GLY:O	2:6:104:MET:HG3	1.99	0.61
15:T:2:GLU:OE1	15:T:2:GLU:N	2.26	0.61
1:AA:160:ALA:O	1:AA:164:THR:HG23	2.01	0.61
5:2:232:THR:C	20:R:269:ARG:HH11	2.08	0.61
9:Av:49:LEU:HB3	29:Av:101:BCR:H14C	1.83	0.61
13:A1:5:ILE:H	13:A1:5:ILE:HD12	1.65	0.61
29:BE:601:BCR:HC21	32:R:411:SQD:H222	1.82	0.61
20:BD:324:ALA:O	20:BD:327:GLY:N	2.32	0.61
13:M:5:ILE:HD12	13:M:5:ILE:H	1.66	0.61
28:9:619:XAT:H241	23:0:601:CHL:C2C	2.31	0.61
26:Ba:318:NEX:H192	26:Ba:318:NEX:H183	1.81	0.61
5:D:108:LEU:HD21	6:E:76:LEU:HD11	1.83	0.61
8:N:226:MET:HE3	25:N:616:LUT:H10	1.83	0.61
4:b:42:LEU:HD11	4:b:93:TYR:HB2	1.83	0.61
5:d:265:LYS:HZ3	20:a:245:THR:H	1.48	0.61
2:0:172:GLY:C	1:AA:62:PHE:CZ	2.79	0.61
24:v:604:CLA:HBB1	24:v:607:CLA:HAB	1.82	0.61
5:2:273:LEU:HD12	20:R:217:SER:HB2	1.83	0.61
15:A7:6:TYR:O	15:A7:10:LEU:HG	1.99	0.61
4:BE:462:PHE:HE1	24:BE:612:CLA:HAB	1.66	0.61
8:Ba:100:VAL:HG11	8:Ba:190:LEU:HD23	1.83	0.61
34:BD:401:DGD:HBH2	32:BD:412:SQD:H341	1.82	0.61
5:D:85:SER:O	16:U:102:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:83:ALA:HA	16:u:86:LYS:NZ	2.15	0.61
23:y:310:CHL:C9	23:y:310:CHL:C11	2.79	0.61
26:y:318:NEX:H192	26:y:318:NEX:H183	1.82	0.61
23:Ba:307:CHL:HBB1	25:Ba:317:LUT:H161	1.83	0.61
27:Y:319:LHG:H281	27:Y:319:LHG:HC91	1.83	0.61
8:g:206:GLU:O	8:g:210:GLU:HG2	2.01	0.61
21:c:76:VAL:HG12	21:c:79:LYS:NZ	2.16	0.61
23:r:606:CHL:HED3	23:r:606:CHL:H11	1.83	0.61
5:BG:350:GLY:HA2	20:BD:334:ARG:HG3	1.83	0.61
23:BQ:609:CHL:C9	23:BQ:609:CHL:C11	2.79	0.61
23:BU:605:CHL:H191	23:BU:607:CHL:H142	1.83	0.61
24:5:610:CLA:H52	25:5:615:LUT:H28	1.83	0.60
8:G:91:THR:HG22	8:G:95:ASN:HD21	1.66	0.60
24:0:613:CLA:HMB2	25:0:615:LUT:H162	1.83	0.60
4:v:384:ARG:HH11	20:R:334:ARG:HH21	1.49	0.60
5:2:85:SER:O	16:A8:102:ARG:NH2	2.33	0.60
12:BO:34:ASN:HD21	20:BD:77:ILE:HB	1.66	0.60
8:BQ:92:PHE:O	8:BQ:96:ARG:HG3	2.01	0.60
4:B:258:TYR:HE2	34:H:102:DGD:HG12	1.66	0.60
24:G:603:CLA:HBC1	23:G:609:CHL:HAC2	1.83	0.60
24:b:603:CLA:HAA1	9:h:57:ILE:HD11	1.83	0.60
8:g:169:MET:HE1	23:g:609:CHL:C1C	2.31	0.60
13:m:7:ALA:O	13:m:11:THR:HG23	2.01	0.60
13:A1:1:MET:HE3	13:A1:2:GLU:N	2.16	0.60
15:A7:1:MET:N	15:A7:1:MET:SD	2.74	0.60
23:Ba:310:CHL:C9	23:Ba:310:CHL:C11	2.79	0.60
3:8:222:GLU:N	3:8:222:GLU:OE1	2.28	0.60
8:y:161:ILE:HD11	23:y:307:CHL:C1D	2.30	0.60
1:9:226:MET:SD	25:9:616:LUT:H10	2.40	0.60
3:AB:188:TYR:HD2	3:AB:214:TYR:HB3	1.66	0.60
5:2:108:LEU:HD21	6:3:76:LEU:HD11	1.83	0.60
5:2:266:ARG:CZ	5:2:270:PHE:HB2	2.32	0.60
6:3:74:GLU:O	6:3:78:GLU:HG2	2.02	0.60
3:8:175:ALA:HA	24:r:601:CLA:HBB2	1.84	0.60
8:N:228:GLY:O	8:N:232:GLN:HG3	2.02	0.60
8:n:111:LEU:HD11	8:n:115:PHE:HD1	1.64	0.60
22:r:141:LEU:HD13	22:r:216:LEU:HD11	1.83	0.60
28:Au:619:XAT:H14	27:A2:618:LHG:H191	1.82	0.60
8:BB:171:ALA:O	8:BB:175:TYR:HD2	1.84	0.60
5:BG:53:THR:HG22	5:BG:68:TYR:HE1	1.66	0.60
20:R:88:ALA:HA	21:1:356:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:107:MET:HE1	24:9:610:CLA:CAB	2.32	0.60
8:A2:226:MET:HE3	25:A2:616:LUT:H10	1.84	0.60
8:BB:60:GLY:HA3	23:BB:302:CHL:HBB1	1.84	0.60
8:BQ:219:GLY:O	8:BQ:223:MET:HG2	2.00	0.60
23:BQ:601:CHL:C9	23:BQ:601:CHL:H112	2.31	0.60
1:5:158:ILE:HG12	2:6:255:TRP:CH2	2.37	0.60
3:8:224:LEU:HD13	24:8:308:CLA:CMA	2.26	0.60
5:D:273:LEU:HD12	20:A:217:SER:HB2	1.82	0.60
6:e:69:ARG:HB2	16:u:102:ARG:HH12	1.67	0.60
24:9:603:CLA:H91	23:9:609:CHL:H142	1.82	0.60
2:6:160:LEU:HD22	23:6:607:CHL:HBC1	1.84	0.60
2:6:164:VAL:HG23	23:6:609:CHL:HBB2	1.84	0.60
4:v:294:GLU:HG2	4:v:296:GLN:HE22	1.67	0.60
27:BB:319:LHG:HC91	27:BB:319:LHG:H281	1.83	0.60
29:8:313:BCR:H403	29:8:313:BCR:H371	1.84	0.60
17:W:124:GLU:OE1	17:W:124:GLU:N	2.34	0.60
24:b:609:CLA:CAB	5:d:124:ILE:HD13	2.32	0.60
5:BG:156:SER:HA	5:BG:160:ILE:HD11	1.83	0.60
23:BQ:606:CHL:HBB1	25:BQ:616:LUT:H161	1.82	0.60
18:X:78:GLY:O	18:X:80:SER:N	2.32	0.60
23:Y:307:CHL:HBB1	25:Y:317:LUT:H161	1.82	0.60
12:l:34:ASN:HD21	20:a:77:ILE:HB	1.65	0.60
13:m:5:ILE:O	13:m:9:ILE:HD12	2.01	0.60
23:n:601:CHL:C9	23:n:601:CHL:C11	2.79	0.60
22:r:144:GLY:O	22:r:148:MET:HB2	2.02	0.60
22:r:170:LYS:HZ1	23:r:606:CHL:CAD	2.14	0.60
3:AB:156:VAL:HG11	23:AB:306:CHL:HMA3	1.83	0.60
4:v:258:TYR:HE2	34:Av:102:DGD:HG12	1.66	0.60
21:BF:41:ARG:HB2	24:BF:512:CLA:HED1	1.84	0.60
10:I:4:LEU:O	10:I:8:VAL:HG13	2.02	0.60
21:C:142:GLU:OE2	21:C:142:GLU:N	2.30	0.60
3:AB:160:ARG:NH2	23:AB:307:CHL:O1D	2.34	0.60
9:Av:21:LYS:HA	9:Av:24:LYS:HG2	1.83	0.60
5:BG:265:LYS:NZ	20:BD:246:TYR:CE1	2.70	0.60
1:7:55:ARG:O	1:7:57:LYS:NZ	2.24	0.59
5:d:265:LYS:CE	20:a:245:THR:HG22	2.30	0.59
8:n:201:LEU:HD12	24:n:610:CLA:H11	1.84	0.59
3:AB:110:MET:HA	3:AB:113:VAL:HG12	1.84	0.59
8:A2:165:GLN:HG3	23:A2:606:CHL:HMA3	1.83	0.59
23:5:607:CHL:C9	23:5:607:CHL:H61	2.32	0.59
1:7:163:ALA:O	1:7:167:ILE:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:25:MET:HE1	29:b:618:BCR:C25	2.32	0.59
4:b:384:ARG:NH1	20:a:334:ARG:HE	2.00	0.59
24:b:610:CLA:C3B	29:h:101:BCR:H323	2.32	0.59
1:9:103:SER:HB2	1:9:219:GLY:HA3	1.85	0.59
13:BP:5:ILE:O	13:BP:9:ILE:HD12	2.01	0.59
6:E:69:ARG:HB2	16:U:102:ARG:HH21	1.67	0.59
8:Y:60:GLY:HA3	23:Y:302:CHL:HBB1	1.83	0.59
5:d:25:ARG:HH21	5:d:26:ASP:HB3	1.67	0.59
1:AA:108:LEU:HD13	24:AA:305:CLA:HBB2	1.84	0.59
3:AB:92:PRO:HA	3:AB:95:LEU:HD12	1.84	0.59
3:AB:108:TRP:CD1	23:AB:307:CHL:HMD3	2.36	0.59
3:AB:222:GLU:HA	3:AB:225:LYS:HG3	1.83	0.59
5:2:85:SER:HB2	16:A8:102:ARG:HH22	1.66	0.59
8:BJ:206:GLU:O	8:BJ:210:GLU:HG2	2.01	0.59
23:BV:605:CHL:HMC	23:BV:606:CHL:C4C	2.33	0.59
2:6:104:MET:HE1	24:6:610:CLA:CAB	2.33	0.59
2:6:224:MET:CG	25:6:616:LUT:H12	2.30	0.59
5:D:194:LEU:O	12:L:35:TYR:OH	2.19	0.59
23:n:609:CHL:C9	23:n:609:CHL:C11	2.79	0.59
2:0:100:GLY:O	2:0:104:MET:HG3	2.02	0.59
5:BG:153:VAL:O	5:BG:157:VAL:HG12	2.02	0.59
20:R:188:ALA:HB2	20:R:328:MET:HE2	1.83	0.59
22:BU:214:LYS:HD3	22:BU:218:PRO:HA	1.84	0.59
33:f:102:HEM:HBC2	33:f:102:HEM:HMC2	1.84	0.59
14:s:230:ARG:HA	14:s:233:MET:HE2	1.84	0.59
23:y:307:CHL:HBB1	25:y:317:LUT:H161	1.84	0.59
23:9:607:CHL:C9	23:9:607:CHL:H61	2.32	0.59
24:9:610:CLA:H52	25:9:615:LUT:H28	1.84	0.59
14:A6:170:ASN:OD1	14:A6:173:LEU:HD12	2.03	0.59
33:BI:102:HEM:HMC2	33:BI:102:HEM:HBC2	1.84	0.59
8:BQ:201:LEU:HD12	24:BQ:610:CLA:H11	1.83	0.59
21:1:87:ILE:C	21:1:90:PRO:HD2	2.27	0.59
20:BD:131:TRP:HZ2	21:BF:449:ARG:HD2	1.66	0.59
22:BU:127:TYR:OH	22:BU:215:ARG:NH1	2.35	0.59
2:6:179:ASP:HB3	14:BV:102:LYS:HD2	1.83	0.59
23:G:601:CHL:C10	23:G:601:CHL:C6	2.81	0.59
1:9:76:GLY:HA3	1:9:216:LEU:HD13	1.84	0.59
24:v:616:CLA:H172	29:v:619:BCR:H331	1.84	0.59
14:A6:118:ALA:O	14:A6:122:MET:HG3	2.03	0.59
18:BA:78:GLY:O	18:BA:80:SER:N	2.31	0.59
23:y:302:CHL:C9	23:y:302:CHL:C11	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:209:LEU:HD21	24:0:610:CLA:H3A	1.83	0.59
8:BJ:236:THR:HG23	8:BJ:238:LYS:H	1.66	0.59
12:BO:24:LEU:O	12:BO:28:LEU:HD23	2.01	0.59
21:BF:396:MET:SD	21:BF:397:THR:HG23	2.42	0.59
22:BU:199:ILE:HA	22:BU:202:ILE:HG22	1.83	0.59
1:5:176:ARG:HH12	23:5:609:CHL:HED1	1.67	0.59
2:6:224:MET:HE1	2:6:227:PHE:HD2	1.67	0.59
3:8:155:TRP:O	3:8:159:LYS:HG2	2.02	0.59
23:n:606:CHL:HBB2	23:n:607:CHL:HBB1	1.84	0.59
3:AB:241:ILE:HD13	25:AB:311:LUT:H42	1.84	0.59
8:Au:219:GLY:O	8:Au:223:MET:HG3	2.02	0.59
17:A0:96:LEU:HA	17:A0:101:LEU:HD12	1.84	0.59
22:BU:240:LEU:HD11	22:BU:244:LYS:HE3	1.83	0.59
2:6:221:MET:CE	24:6:602:CLA:HHC	2.33	0.59
3:8:100:GLU:HG3	3:8:192:GLN:OE1	2.02	0.59
28:G:619:XAT:H14	27:N:618:LHG:H191	1.84	0.59
12:L:27:VAL:HG21	27:L:102:LHG:H192	1.85	0.59
8:Y:110:ALA:HA	8:Y:226:MET:HE1	1.84	0.59
23:y:302:CHL:HHC	23:y:302:CHL:HBB1	1.84	0.59
17:A0:110:GLY:O	17:A0:114:THR:HG23	2.03	0.59
8:Ba:163:ALA:O	8:Ba:167:ILE:HG12	2.03	0.59
23:Ba:302:CHL:HHC	23:Ba:302:CHL:HBB1	1.85	0.59
24:BF:513:CLA:H91	27:BF:521:LHG:H341	1.84	0.59
23:BU:606:CHL:C10	23:BU:606:CHL:C6	2.80	0.59
17:W:110:GLY:O	17:W:114:THR:HG23	2.03	0.59
27:g:618:LHG:HC41	28:y:301:XAT:H363	1.85	0.59
23:s:605:CHL:HMC	23:s:606:CHL:C4C	2.32	0.59
21:c:138:GLU:OE2	21:c:138:GLU:N	2.24	0.59
8:A2:226:MET:HG3	25:A2:616:LUT:H12	1.83	0.59
8:BJ:94:ARG:O	8:BJ:98:LEU:HD12	2.03	0.59
23:BQ:601:CHL:C9	23:BQ:601:CHL:C11	2.81	0.59
34:BF:518:DGD:HD3	30:BF:519:LMG:HC1	1.84	0.59
24:B:601:CLA:H102	29:H:101:BCR:H402	1.85	0.58
5:D:85:SER:HB2	16:U:102:ARG:HH22	1.66	0.58
5:d:160:ILE:HD11	5:d:288:VAL:HG22	1.85	0.58
20:a:226:GLU:N	20:a:226:GLU:OE2	2.36	0.58
21:c:78:GLU:CB	21:c:79:LYS:HZ2	2.14	0.58
34:c:517:DGD:HD3	30:c:518:LMG:HC1	1.85	0.58
8:Au:238:LYS:HG3	8:Au:242:GLU:HB2	1.85	0.58
14:BV:103:LYS:HD3	14:BV:106:ASN:HD22	1.67	0.58
27:Ba:319:LHG:HC91	27:Ba:319:LHG:H281	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:58:TYR:CD2	23:7:302:CHL:HAA1	2.39	0.58
8:G:219:GLY:O	8:G:223:MET:HG3	2.03	0.58
8:g:94:ARG:O	8:g:98:LEU:HD12	2.03	0.58
8:g:236:THR:HG23	8:g:238:LYS:H	1.67	0.58
23:r:605:CHL:H191	23:r:607:CHL:H142	1.84	0.58
23:r:606:CHL:C10	23:r:606:CHL:C6	2.81	0.58
3:AB:110:MET:SD	24:AB:308:CLA:HMC3	2.43	0.58
24:Ba:311:CLA:CHB	24:Ba:311:CLA:H2	2.33	0.58
33:F:102:HEM:HBB2	33:F:102:HEM:HMB2	1.85	0.58
27:y:319:LHG:H281	27:y:319:LHG:HC91	1.84	0.58
1:AA:58:TYR:CD2	23:AA:302:CHL:HAA1	2.37	0.58
24:v:601:CLA:H102	29:Av:101:BCR:H402	1.86	0.58
10:BL:31:ASN:OD1	10:BL:33:GLY:N	2.34	0.58
1:5:138:ILE:HD11	1:5:158:ILE:HB	1.85	0.58
8:G:169:MET:HE1	23:G:609:CHL:C1C	2.33	0.58
8:N:191:TYR:HD2	24:N:610:CLA:O1D	1.86	0.58
23:Y:302:CHL:HBB1	23:Y:302:CHL:HHC	1.85	0.58
24:b:610:CLA:C3D	9:h:43:MET:HE1	2.34	0.58
5:d:90:LEU:H	5:d:90:LEU:HD12	1.68	0.58
20:a:100:ALA:N	20:a:104:GLU:OE1	2.36	0.58
23:r:605:CHL:HMC	23:r:606:CHL:C2C	2.33	0.58
23:0:609:CHL:HHC	23:0:609:CHL:HBB1	1.86	0.58
3:AB:155:TRP:O	3:AB:159:LYS:HG2	2.03	0.58
8:A2:206:GLU:O	8:A2:210:GLU:HG2	2.03	0.58
4:BE:42:LEU:HD11	4:BE:93:TYR:HB2	1.84	0.58
24:BE:603:CLA:H202	34:BK:102:DGD:HAW1	1.86	0.58
5:BG:151:ILE:O	5:BG:155:VAL:HG13	2.03	0.58
27:BJ:618:LHG:HC41	28:Ba:301:XAT:H363	1.85	0.58
23:BQ:608:CHL:HBD	23:BQ:608:CHL:HBA1	1.86	0.58
24:6:613:CLA:H12	24:6:614:CLA:C3D	2.34	0.58
8:BB:197:ASP:OD2	8:BB:200:GLY:N	2.36	0.58
20:BD:183:MET:CE	24:BD:406:CLA:HHD	2.34	0.58
22:BU:83:LEU:HD23	24:BU:602:CLA:H42	1.86	0.58
24:5:603:CLA:H91	23:5:609:CHL:H142	1.86	0.58
14:S:135:ASN:ND2	14:S:141:CYS:HB3	2.18	0.58
29:b:601:BCR:HC21	32:A:413:SQD:H222	1.85	0.58
22:r:240:LEU:HD11	22:r:244:LYS:HE3	1.86	0.58
22:r:284:ILE:HA	22:r:287:PHE:HB3	1.85	0.58
1:AA:165:GLN:HG3	23:AA:307:CHL:HMA3	1.86	0.58
3:AB:221:LEU:O	3:AB:225:LYS:HG3	2.03	0.58
4:v:203:ILE:O	4:v:207:THR:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:18:ILE:HG13	18:BA:110:PHE:CD2	2.39	0.58
8:BB:250:ASP:HB3	8:BB:254:ASN:OD1	2.03	0.58
8:BJ:113:CYS:HG	8:BJ:131:TRP:CG	2.21	0.58
8:Ba:141:ASP:OD1	8:Ba:142:GLY:N	2.36	0.58
8:Y:171:ALA:O	8:Y:175:TYR:HD2	1.87	0.58
5:d:322:LEU:O	5:d:326:ILE:HG13	2.02	0.58
23:g:601:CHL:H52	23:y:310:CHL:HHC	1.86	0.58
8:y:163:ALA:O	8:y:167:ILE:HG12	2.03	0.58
24:0:613:CLA:H12	24:0:614:CLA:C3D	2.33	0.58
3:AB:106:GLY:HA3	3:AB:232:SER:HB3	1.85	0.58
3:AB:110:MET:SD	3:AB:111:ALA:N	2.76	0.58
3:AB:238:ALA:HA	25:AB:311:LUT:H182	1.85	0.58
6:3:69:ARG:HB2	16:A8:102:ARG:HH21	1.67	0.58
23:BB:302:CHL:H41	27:BB:319:LHG:H192	1.86	0.58
8:BJ:73:GLU:OE1	8:BJ:73:GLU:N	2.31	0.58
23:BQ:601:CHL:HHC	23:BQ:601:CHL:HBB1	1.85	0.58
23:BU:606:CHL:HED3	23:BU:606:CHL:H11	1.85	0.58
6:E:74:GLU:O	6:E:78:GLU:HG2	2.04	0.58
14:S:189:ARG:NH2	24:S:608:CLA:O1D	2.36	0.58
8:Y:250:ASP:HB3	8:Y:254:ASN:OD1	2.04	0.58
14:s:207:ASP:OD1	25:s:614:LUT:O23	2.21	0.58
24:9:604:CLA:HBA1	23:9:606:CHL:CHD	2.33	0.58
1:AA:93:ALA:HA	1:AA:96:ARG:HG3	1.86	0.58
23:Au:601:CHL:C10	23:Au:601:CHL:C6	2.81	0.58
14:A6:67:ARG:NE	14:A6:92:ASP:OD1	2.37	0.58
10:I:1:MET:HE3	30:I:101:LMG:HC5	1.85	0.58
15:T:14:LEU:O	15:T:17:ILE:HG22	2.04	0.58
4:b:366:PHE:HB3	4:b:425:GLN:NE2	2.19	0.58
5:d:102:PHE:HE2	6:e:47:PHE:HE2	1.50	0.58
17:w:84:ARG:NH1	20:a:97:TRP:C	2.59	0.58
19:z:9:VAL:O	19:z:13:ILE:HG12	2.04	0.58
2:0:245:HIS:HB2	24:0:613:CLA:HAA2	1.86	0.58
1:AA:78:TYR:N	24:AA:303:CLA:OBD	2.37	0.58
27:Au:618:LHG:HC41	28:BB:301:XAT:H363	1.84	0.58
4:BE:30:VAL:HG12	24:BE:606:CLA:HHD	1.85	0.58
4:BE:66:MET:HE2	24:BE:606:CLA:HED3	1.84	0.58
19:Bb:9:VAL:O	19:Bb:13:ILE:HG12	2.04	0.58
24:5:604:CLA:HBA1	23:5:606:CHL:CHD	2.34	0.58
2:6:229:VAL:HG21	24:6:613:CLA:HAC2	1.86	0.58
24:6:613:CLA:HMB3	25:6:615:LUT:H162	1.85	0.58
12:L:24:LEU:O	12:L:28:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:121:GLU:O	9:h:24:LYS:NZ	2.21	0.58
33:f:102:HEM:HBB2	33:f:102:HEM:HMB1	1.86	0.58
33:4:102:HEM:HBB2	33:4:102:HEM:HMB2	1.85	0.58
11:Ay:28:GLU:CD	11:Ay:28:GLU:H	2.11	0.58
24:BE:603:CLA:HAA1	9:BK:57:ILE:HD11	1.85	0.58
21:1:456:GLU:OE2	21:1:456:GLU:N	2.28	0.58
1:7:58:TYR:HD2	23:7:302:CHL:HAA1	1.68	0.57
16:U:82:GLU:OE1	16:U:82:GLU:N	2.35	0.57
8:Y:160:ALA:O	8:Y:164:THR:HG22	2.03	0.57
23:Y:302:CHL:H41	27:Y:319:LHG:H192	1.86	0.57
24:C:513:CLA:HBA1	24:C:513:CLA:HBD	1.84	0.57
20:a:183:MET:CE	24:a:406:CLA:HHD	2.34	0.57
22:r:134:GLN:NE2	22:r:135:ARG:HG2	2.19	0.57
24:9:602:CLA:H12	24:9:602:CLA:H3A	1.86	0.57
3:AB:140:PHE:HD2	3:AB:145:LEU:HD22	1.69	0.57
4:v:55:MET:HG3	4:v:60:MET:HB2	1.84	0.57
14:BV:123:LEU:HD12	24:BV:604:CLA:HMC3	1.85	0.57
20:R:183:MET:CE	24:R:405:CLA:HHD	2.34	0.57
23:BU:605:CHL:HMC	23:BU:606:CHL:C2C	2.34	0.57
2:0:224:MET:HE1	2:0:227:PHE:HD2	1.68	0.57
27:BJ:618:LHG:H211	28:Ba:301:XAT:H12	1.86	0.57
21:BF:83:GLU:OE2	21:BF:398:HIS:NE2	2.32	0.57
2:6:170:VAL:HA	2:6:173:PHE:CD1	2.40	0.57
8:G:217:LYS:HZ3	24:G:611:CLA:CGD	2.17	0.57
19:Z:42:SER:O	19:Z:46:LEU:HG	2.03	0.57
4:b:30:VAL:HG12	24:b:606:CLA:HHD	1.84	0.57
23:n:601:CHL:HBB1	23:n:601:CHL:HHC	1.85	0.57
23:n:608:CHL:HBD	23:n:608:CHL:HBA1	1.85	0.57
8:y:76:GLY:HA3	8:y:216:LEU:HD23	1.86	0.57
38:A:408:PHO:H41	32:A:413:SQD:H223	1.85	0.57
20:a:333:GLU:HB3	20:a:336:ALA:HB2	1.86	0.57
21:c:81:MET:HG3	21:c:86:LEU:HD12	1.86	0.57
23:r:605:CHL:HMC	23:r:606:CHL:C4C	2.33	0.57
2:0:199:LEU:HD11	2:0:209:LEU:HD22	1.86	0.57
3:AB:116:ILE:O	3:AB:120:GLN:HG2	2.04	0.57
1:7:103:SER:HB2	1:7:219:GLY:HA3	1.86	0.57
9:h:40:THR:HA	9:h:43:MET:HG2	1.86	0.57
20:A:153:ALA:O	20:A:157:VAL:HG12	2.04	0.57
21:C:318:LEU:HD12	21:C:340:TYR:HB3	1.86	0.57
23:r:607:CHL:C9	23:r:607:CHL:H112	2.35	0.57
1:9:138:ILE:HD13	1:9:158:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:384:ARG:HD3	5:2:353:LEU:HD13	1.86	0.57
24:A2:610:CLA:H42	25:A2:615:LUT:H26	1.86	0.57
14:BV:181:LEU:HD22	26:BV:616:NEX:H15	1.87	0.57
20:BD:195:HIS:CD2	20:BD:293:MET:HE2	2.40	0.57
2:6:208:GLU:O	2:6:212:LYS:HG2	2.04	0.57
3:8:146:LEU:O	3:8:150:LEU:HG	2.03	0.57
5:D:153:VAL:HG22	24:D:401:CLA:HED3	1.84	0.57
8:N:206:GLU:O	8:N:210:GLU:HG2	2.03	0.57
24:c:513:CLA:H91	27:c:520:LHG:H341	1.84	0.57
3:AB:140:PHE:CE1	22:BU:279:LEU:HD13	2.40	0.57
8:BB:160:ALA:O	8:BB:164:THR:HG22	2.04	0.57
8:BJ:219:GLY:O	8:BJ:223:MET:HG3	2.04	0.57
13:BP:9:ILE:HD12	13:BP:9:ILE:H	1.69	0.57
3:8:251:THR:HG23	3:8:254:GLY:H	1.69	0.57
14:s:99:GLY:HA3	2:0:179:ASP:OD2	2.05	0.57
34:C:517:DGD:HD3	30:C:519:LMG:HC1	1.85	0.57
17:A0:125:GLU:OE1	21:1:262:ARG:NH1	2.31	0.57
5:BG:150:PRO:HA	5:BG:153:VAL:HG12	1.84	0.57
9:BK:40:THR:HA	9:BK:43:MET:HG2	1.86	0.57
22:r:83:LEU:HD23	24:r:602:CLA:H42	1.86	0.57
24:AA:304:CLA:CAD	23:AA:310:CHL:H2	2.35	0.57
8:BJ:196:PHE:O	25:BJ:615:LUT:H24	2.04	0.57
2:6:135:GLN:O	2:6:138:SER:OG	2.23	0.57
2:6:230:GLN:HE22	24:6:613:CLA:C1D	2.18	0.57
3:8:99:ARG:NH2	3:8:102:GLU:OE1	2.38	0.57
8:N:58:TYR:CZ	8:N:59:LEU:HD21	2.40	0.57
25:S:615:LUT:H8	25:S:615:LUT:C17	2.31	0.57
20:a:134:SER:HA	20:a:139:MET:HE2	1.87	0.57
4:BE:55:MET:HG2	4:BE:60:MET:HB2	1.86	0.57
8:BJ:231:VAL:HG11	24:BJ:613:CLA:HAC2	1.86	0.57
21:BF:342:MET:HE2	21:BF:352:GLY:HA2	1.87	0.57
22:BU:170:LYS:NZ	23:BU:606:CHL:OBD	2.37	0.57
28:5:619:XAT:H381	28:5:619:XAT:H393	1.87	0.57
2:6:179:ASP:OD1	14:BV:99:GLY:HA3	2.05	0.57
3:8:238:ALA:HA	25:8:311:LUT:H182	1.87	0.57
27:G:618:LHG:HC41	28:Y:301:XAT:H363	1.86	0.57
17:W:128:GLU:N	17:W:128:GLU:OE2	2.37	0.57
17:W:133:LEU:HD12	17:W:133:LEU:N	2.18	0.57
19:Z:4:ALA:O	19:Z:7:LEU:HD12	2.05	0.57
21:c:83:GLU:OE2	21:c:398:HIS:NE2	2.29	0.57
22:r:188:ILE:H	22:r:188:ILE:HD12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:58:TYR:HD2	23:AA:302:CHL:HAA1	1.68	0.57
4:BE:384:ARG:NH1	20:BD:334:ARG:HE	2.02	0.57
33:BI:102:HEM:HBB2	33:BI:102:HEM:HMB1	1.87	0.57
24:BD:405:CLA:HBD	24:BD:406:CLA:HAC2	1.86	0.57
23:N:609:CHL:HBB1	23:Y:302:CHL:H51	1.86	0.57
14:S:246:THR:HG23	14:S:248:GLU:H	1.70	0.57
15:T:1:MET:SD	15:T:1:MET:N	2.63	0.57
8:g:100:VAL:O	8:g:103:SER:OG	2.19	0.57
9:h:47:MET:HE1	29:h:101:BCR:H312	1.86	0.57
21:C:87:ILE:C	21:C:90:PRO:HD2	2.30	0.57
24:r:612:CLA:HMB2	25:r:615:LUT:H162	1.86	0.57
3:AB:251:THR:HG23	3:AB:254:GLY:H	1.70	0.57
21:1:342:MET:HE3	21:1:343:ARG:HB2	1.85	0.57
34:1:517:DGD:HD3	30:1:519:LMG:HC1	1.85	0.57
1:7:93:ALA:HA	1:7:96:ARG:HG3	1.87	0.56
3:8:116:ILE:O	3:8:120:GLN:HG2	2.05	0.56
24:8:302:CLA:HBC3	28:8:312:XAT:H12	1.86	0.56
15:T:8:PHE:HE1	29:b:601:BCR:H361	1.69	0.56
9:h:49:LEU:HB3	29:h:101:BCR:H14C	1.86	0.56
9:h:60:ILE:HA	9:h:65:VAL:HG12	1.87	0.56
24:r:609:CLA:H2	25:r:615:LUT:H373	1.86	0.56
2:0:237:GLY:O	2:0:241:ASN:ND2	2.38	0.56
1:AA:165:GLN:O	1:AA:169:MET:HG3	2.04	0.56
4:BE:366:PHE:HB3	4:BE:425:GLN:NE2	2.20	0.56
29:BE:601:BCR:HC41	32:R:411:SQD:H202	1.87	0.56
23:BJ:601:CHL:C10	23:BJ:601:CHL:C6	2.83	0.56
20:R:183:MET:HE2	24:R:405:CLA:HAC1	1.86	0.56
24:B:604:CLA:HBB1	24:B:607:CLA:HAB	1.87	0.56
11:K:28:GLU:CD	11:K:28:GLU:H	2.14	0.56
19:z:3:ILE:O	19:z:7:LEU:HG	2.05	0.56
21:c:26:ARG:HH12	24:c:512:CLA:CBD	2.17	0.56
3:AB:176:THR:OG1	3:AB:179:SER:O	2.23	0.56
19:BC:3:ILE:O	19:BC:7:LEU:HG	2.04	0.56
19:BC:57:LEU:HD22	19:BC:60:LEU:HD21	1.87	0.56
20:R:153:ALA:O	20:R:157:VAL:HG12	2.04	0.56
2:6:221:MET:CE	24:6:602:CLA:HAB	2.35	0.56
1:7:78:TYR:N	24:7:303:CLA:OBD	2.37	0.56
1:7:165:GLN:HG3	23:7:307:CHL:HMA3	1.87	0.56
1:7:208:PHE:O	1:7:212:LYS:HG2	2.06	0.56
24:7:304:CLA:CAD	23:7:310:CHL:H2	2.35	0.56
24:B:606:CLA:H3A	24:B:606:CLA:CGA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:616:CLA:H172	29:B:619:BCR:H331	1.86	0.56
5:D:18:ILE:HG13	18:X:110:PHE:CD2	2.39	0.56
13:M:1:MET:HE3	13:M:2:GLU:H	1.70	0.56
17:W:84:ARG:NH1	17:W:86:SER:OG	2.38	0.56
8:Y:103:SER:HB2	8:Y:219:GLY:HA3	1.87	0.56
4:b:223:GLN:HE22	9:h:34:ALA:C	2.13	0.56
27:b:624:LHG:H192	12:l:27:VAL:HG21	1.87	0.56
8:g:149:ASN:HB3	8:g:152:LEU:HG	1.88	0.56
21:c:240:LEU:HD23	21:c:244:CYS:SG	2.46	0.56
22:r:67:TRP:HD1	22:r:68:LEU:HG	1.70	0.56
22:r:126:PRO:HG2	22:r:127:TYR:HD1	1.71	0.56
24:r:602:CLA:H101	28:r:616:XAT:H28	1.87	0.56
1:9:163:ALA:O	1:9:167:ILE:HG22	2.05	0.56
2:0:91:LYS:NZ	1:AA:83:ALA:HA	2.20	0.56
5:2:47:GLY:O	5:2:51:THR:HG22	2.06	0.56
19:BC:1:MET:HE1	19:BC:61:ILE:HB	1.86	0.56
24:BE:617:CLA:H172	29:BE:620:BCR:H331	1.86	0.56
23:BJ:606:CHL:HMC	25:BJ:616:LUT:H163	1.88	0.56
8:Ba:76:GLY:HA3	8:Ba:216:LEU:HD23	1.87	0.56
8:G:169:MET:HA	8:G:172:VAL:HG12	1.87	0.56
29:b:601:BCR:HC41	32:A:413:SQD:H202	1.86	0.56
13:m:9:ILE:HD12	13:m:9:ILE:H	1.70	0.56
21:c:41:ARG:HB2	24:c:512:CLA:HED1	1.86	0.56
23:A2:609:CHL:C9	23:A2:609:CHL:C11	2.83	0.56
8:BB:103:SER:O	8:BB:107:MET:HG3	2.05	0.56
38:R:407:PHO:H41	32:R:411:SQD:H223	1.86	0.56
3:8:153:MET:HE2	3:8:157:GLU:CD	2.31	0.56
24:B:607:CLA:HAC2	29:B:623:BCR:H272	1.87	0.56
5:2:228:ASP:OD1	5:2:228:ASP:N	2.37	0.56
8:A2:58:TYR:CZ	8:A2:59:LEU:HD21	2.41	0.56
19:Bb:3:ILE:O	19:Bb:7:LEU:HG	2.06	0.56
23:BU:607:CHL:C9	23:BU:607:CHL:H112	2.35	0.56
24:7:303:CLA:HMB2	24:7:303:CLA:H51	1.87	0.56
4:B:92:SER:OG	4:B:94:GLU:OE1	2.18	0.56
27:b:623:LHG:O4	5:d:142:TYR:OH	2.23	0.56
6:e:74:GLU:O	6:e:78:GLU:HG2	2.06	0.56
7:f:27:PHE:O	7:f:31:ILE:HG22	2.06	0.56
8:g:113:CYS:HG	8:g:131:TRP:CG	2.23	0.56
8:y:90:GLU:O	8:y:94:ARG:HG2	2.05	0.56
24:A:405:CLA:C2	38:A:408:PHO:HBB1	2.36	0.56
21:C:443:TRP:HE1	24:C:508:CLA:HED3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:104:MET:HE1	24:0:610:CLA:CAB	2.35	0.56
2:0:135:GLN:O	2:0:138:SER:OG	2.23	0.56
23:Au:607:CHL:HHC	23:Au:607:CHL:HBB1	1.87	0.56
8:A2:188:ASP:OD2	8:A2:191:TYR:N	2.37	0.56
23:A2:609:CHL:HBB1	23:BB:302:CHL:H51	1.88	0.56
5:BG:53:THR:HG22	5:BG:68:TYR:CE1	2.41	0.56
19:Bb:15:THR:O	19:Bb:19:LEU:HG	2.06	0.56
5:D:321:LEU:HB3	20:A:331:MET:CE	2.36	0.56
7:f:18:HIS:O	7:f:22:VAL:HG23	2.06	0.56
11:Ay:40:MET:HE1	29:Ay:101:BCR:C4	2.36	0.56
6:BH:74:GLU:OE1	6:BH:74:GLU:N	2.34	0.56
8:BJ:149:ASN:HB3	8:BJ:152:LEU:HG	1.88	0.56
21:1:297:TYR:OH	24:1:502:CLA:O1A	2.24	0.56
20:BD:288:LEU:HD21	21:BF:435:PHE:HD2	1.70	0.56
3:8:92:PRO:HA	3:8:95:LEU:HD12	1.88	0.56
8:N:59:LEU:HD22	8:N:59:LEU:N	2.20	0.56
24:N:610:CLA:H42	25:N:615:LUT:H26	1.87	0.56
27:g:618:LHG:H211	28:y:301:XAT:H12	1.87	0.56
14:s:181:LEU:HD22	26:s:616:NEX:H15	1.88	0.56
24:s:609:CLA:H3A	24:s:609:CLA:CGA	2.35	0.56
21:C:45:LEU:HD12	21:C:138:GLU:HB3	1.86	0.56
24:Au:613:CLA:H52	28:BB:301:XAT:H203	1.88	0.56
27:BE:623:LHG:O4	5:BG:142:TYR:OH	2.21	0.56
21:1:443:TRP:HE1	24:1:508:CLA:HED3	1.69	0.56
22:BU:138:GLU:HB3	22:BU:216:LEU:HD21	1.88	0.56
28:5:619:XAT:H382	23:6:601:CHL:NC	2.21	0.56
6:e:68:GLY:O	6:e:72:SER:OG	2.22	0.56
9:h:40:THR:O	9:h:43:MET:HB2	2.05	0.56
8:n:103:SER:O	8:n:107:MET:HG3	2.06	0.56
1:AA:86:SER:HB3	1:AA:92:PHE:HD1	1.70	0.56
25:A6:615:LUT:H8	25:A6:615:LUT:C17	2.31	0.56
5:BG:266:ARG:HE	20:BD:223:LEU:HD11	1.70	0.56
8:BJ:106:ALA:HB3	8:BJ:223:MET:HG2	1.87	0.56
2:6:90:ALA:HA	2:6:93:ARG:NE	2.21	0.56
28:G:619:XAT:H203	24:N:613:CLA:H52	1.88	0.56
5:d:30:PHE:HZ	5:d:132:GLU:OE2	1.88	0.56
8:g:196:PHE:O	25:g:615:LUT:H24	2.04	0.56
23:g:609:CHL:HHC	23:n:601:CHL:H52	1.88	0.56
17:w:125:GLU:OE2	21:c:261:ARG:NH1	2.38	0.56
2:0:229:VAL:HG21	24:0:613:CLA:HAC2	1.87	0.56
23:AB:304:CHL:H3A	29:AB:313:BCR:H21C	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:603:CLA:HAB	24:v:605:CLA:H152	1.88	0.56
5:BG:55:PHE:HD2	6:BH:47:PHE:CE2	2.23	0.56
19:Bb:27:PHE:HB3	21:BF:134:LEU:HD23	1.88	0.56
24:1:512:CLA:H91	27:1:521:LHG:H341	1.88	0.56
20:BD:332:HIS:NE2	36:BD:403:OEX:O5	2.39	0.56
24:BU:609:CLA:H2	25:BU:615:LUT:H373	1.88	0.56
25:5:616:LUT:H181	25:5:616:LUT:H8	1.88	0.55
4:B:106:LEU:HD11	29:B:619:BCR:C16	2.36	0.55
23:G:609:CHL:HBC3	23:G:609:CHL:HMC	1.87	0.55
22:r:189:SER:O	22:r:192:ILE:HG13	2.06	0.55
2:0:167:MET:HE1	23:0:609:CHL:C1C	2.36	0.55
1:AA:78:TYR:HE2	23:AA:302:CHL:HBC2	1.71	0.55
1:AA:208:PHE:O	1:AA:212:LYS:HG2	2.06	0.55
24:v:606:CLA:H3A	24:v:606:CLA:CGA	2.35	0.55
5:2:194:LEU:O	12:Az:35:TYR:OH	2.20	0.55
17:A0:128:GLU:N	17:A0:128:GLU:OE2	2.38	0.55
23:BJ:609:CHL:HHC	23:BQ:601:CHL:H52	1.88	0.55
21:BF:443:TRP:HE1	24:BF:509:CLA:HED3	1.71	0.55
23:G:607:CHL:C10	23:G:607:CHL:C6	2.85	0.55
4:b:55:MET:HG2	4:b:60:MET:HB2	1.89	0.55
23:g:601:CHL:C10	23:g:601:CHL:C6	2.84	0.55
2:0:177:GLY:HA2	23:0:608:CHL:HMC	1.87	0.55
8:BQ:165:GLN:HG3	23:BQ:606:CHL:HMA3	1.87	0.55
22:BU:188:ILE:HD12	22:BU:188:ILE:H	1.71	0.55
2:6:91:LYS:NZ	1:7:83:ALA:HA	2.20	0.55
8:N:166:VAL:HG23	23:N:609:CHL:HBB2	1.88	0.55
24:b:617:CLA:H172	29:b:620:BCR:H331	1.87	0.55
14:s:122:MET:HE3	14:s:229:GLY:CA	2.36	0.55
22:r:192:ILE:O	22:r:196:VAL:HG13	2.05	0.55
1:9:235:VAL:HG23	1:9:236:THR:HG23	1.87	0.55
28:9:619:XAT:H382	23:0:601:CHL:NC	2.21	0.55
4:v:66:MET:HE2	24:v:605:CLA:HED3	1.88	0.55
5:BG:196:PRO:O	5:BG:200:MET:HG3	2.06	0.55
9:BK:40:THR:O	9:BK:43:MET:HB2	2.06	0.55
23:BQ:606:CHL:HBB2	23:BQ:607:CHL:HBB1	1.87	0.55
24:B:605:CLA:HBB1	24:B:606:CLA:H51	1.89	0.55
24:G:613:CLA:H52	28:Y:301:XAT:H203	1.88	0.55
19:Z:1:MET:HE1	19:Z:61:ILE:HB	1.88	0.55
4:b:2:GLY:N	12:l:12:GLU:OE1	2.39	0.55
9:h:66:LEU:HB3	18:x:81:PRO:HG3	1.89	0.55
20:A:201:GLY:HA3	20:A:286:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:288:LEU:HD21	21:c:435:PHE:HD2	1.72	0.55
21:c:367:GLU:HA	21:c:370:ARG:HD2	1.87	0.55
28:Au:619:XAT:H15	24:A2:613:CLA:H102	1.88	0.55
22:BU:67:TRP:HD1	22:BU:68:LEU:HG	1.71	0.55
22:BU:138:GLU:CB	22:BU:216:LEU:HD21	2.36	0.55
1:7:169:MET:HE1	1:7:173:GLU:HG3	1.88	0.55
10:i:31:ASN:OD1	10:i:33:GLY:N	2.38	0.55
24:C:512:CLA:H91	27:C:521:LHG:H341	1.88	0.55
24:9:604:CLA:HMB2	25:9:616:LUT:H162	1.88	0.55
23:9:607:CHL:C9	23:9:607:CHL:C6	2.85	0.55
28:9:619:XAT:H14	27:0:617:LHG:H172	1.89	0.55
5:2:322:LEU:HD13	20:R:184:ILE:HG21	1.87	0.55
18:BZ:94:GLY:O	18:BZ:98:THR:HG23	2.06	0.55
8:Ba:121:ARG:HH12	8:Ba:245:ALA:HB2	1.72	0.55
8:Ba:169:MET:HE1	23:Ba:310:CHL:C1C	2.35	0.55
24:R:404:CLA:C2	38:R:407:PHO:HBB1	2.36	0.55
23:5:607:CHL:C9	23:5:607:CHL:C6	2.84	0.55
25:5:616:LUT:H181	25:5:616:LUT:C8	2.36	0.55
1:7:165:GLN:O	1:7:169:MET:HG3	2.07	0.55
23:r:607:CHL:C9	23:r:607:CHL:C11	2.84	0.55
3:AB:106:GLY:O	3:AB:110:MET:HG3	2.07	0.55
3:AB:139:PRO:O	3:AB:140:PHE:HD1	1.90	0.55
5:2:266:ARG:HH12	20:R:220:THR:CG2	2.20	0.55
6:3:74:GLU:N	6:3:74:GLU:OE1	2.33	0.55
5:BG:84:ASN:ND2	5:BG:166:SER:OG	2.40	0.55
22:BU:194:ILE:O	22:BU:198:VAL:HG22	2.06	0.55
22:BU:207:ASN:HA	22:BU:215:ARG:HH21	1.71	0.55
22:BU:284:ILE:HA	22:BU:287:PHE:HB3	1.88	0.55
25:6:615:LUT:H181	25:6:615:LUT:C8	2.36	0.55
24:Y:312:CLA:HAA1	24:Y:312:CLA:HED2	1.88	0.55
5:d:265:LYS:HE2	20:a:245:THR:CG2	2.34	0.55
24:9:613:CLA:C4C	24:9:613:CLA:H51	2.37	0.55
24:AB:302:CLA:HBC3	28:AB:312:XAT:H12	1.87	0.55
24:BB:312:CLA:HED2	24:BB:312:CLA:HAA1	1.89	0.55
7:BI:18:HIS:O	7:BI:22:VAL:HG23	2.07	0.55
9:BK:49:LEU:HB3	29:BK:101:BCR:H14C	1.87	0.55
21:1:81:MET:HG3	21:1:86:LEU:HD12	1.89	0.55
4:B:315:ILE:HD13	4:B:359:MET:HE2	1.89	0.55
8:Y:219:GLY:O	8:Y:223:MET:HG3	2.06	0.55
5:d:350:GLY:HA2	20:a:334:ARG:HG3	1.89	0.55
14:A6:135:ASN:ND2	14:A6:141:CYS:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:230:ALA:HA	21:BF:457:LYS:HZ3	1.68	0.55
8:BJ:138:ILE:HD13	8:BJ:144:LEU:HD23	1.89	0.55
28:BJ:619:XAT:H203	24:BQ:613:CLA:H52	1.89	0.55
14:BV:239:PHE:HE1	25:BV:614:LUT:H41	1.72	0.55
1:7:78:TYR:HE2	23:7:302:CHL:HBC2	1.72	0.55
1:7:97:GLU:O	1:7:101:ILE:HG22	2.06	0.55
3:8:176:THR:OG1	3:8:179:SER:O	2.19	0.55
24:c:514:CLA:HBD	24:c:514:CLA:HBA1	1.89	0.55
3:AB:188:TYR:CD2	3:AB:214:TYR:HB3	2.41	0.55
3:AB:200:PHE:HB3	24:AB:308:CLA:OBD	2.07	0.55
5:2:322:LEU:HD13	20:R:184:ILE:CG2	2.36	0.55
8:Au:103:SER:O	8:Au:107:MET:HG3	2.07	0.55
28:Au:619:XAT:H203	24:A2:613:CLA:H52	1.89	0.55
8:A2:166:VAL:HG23	23:A2:609:CHL:HBB2	1.89	0.55
23:A2:605:CHL:HMB2	14:A6:137:TYR:OH	2.07	0.55
6:BH:74:GLU:O	6:BH:78:GLU:HG2	2.06	0.55
1:5:235:VAL:HG23	1:5:236:THR:HG23	1.87	0.55
4:B:66:MET:HE2	24:B:605:CLA:HED3	1.89	0.55
8:N:58:TYR:CE2	8:N:59:LEU:HD21	2.42	0.55
24:g:603:CLA:HBC1	23:g:609:CHL:HAC2	1.88	0.55
21:c:104:GLU:N	21:c:104:GLU:OE2	2.34	0.55
24:Au:612:CLA:HMC3	25:Au:615:LUT:H191	1.89	0.55
8:A2:59:LEU:HD22	8:A2:59:LEU:N	2.22	0.55
24:BE:612:CLA:H2A	24:BE:612:CLA:CED	2.37	0.55
24:BJ:603:CLA:HBC1	23:BJ:609:CHL:HAC2	1.88	0.55
4:B:247:PHE:HE1	24:B:602:CLA:H122	1.72	0.54
8:g:138:ILE:HD13	8:g:144:LEU:HD23	1.89	0.54
4:v:223:GLN:HE22	4:v:224:ARG:NH1	2.05	0.54
24:Au:613:CLA:H72	28:BB:301:XAT:H203	1.89	0.54
20:BD:92:HIS:ND1	21:BF:219:GLY:O	2.40	0.54
2:6:245:HIS:HB2	24:6:613:CLA:HAA2	1.90	0.54
4:B:472:ARG:HD3	4:B:479:PHE:CZ	2.42	0.54
14:S:118:ALA:O	14:S:122:MET:HG3	2.06	0.54
8:n:88:ASP:OD2	8:n:90:GLU:HG3	2.08	0.54
8:y:121:ARG:HH12	8:y:245:ALA:HB2	1.73	0.54
20:A:183:MET:CE	24:A:406:CLA:HHD	2.36	0.54
2:0:91:LYS:HZ3	1:AA:83:ALA:HA	1.72	0.54
2:0:224:MET:CG	25:0:616:LUT:H12	2.32	0.54
1:AA:169:MET:HE1	1:AA:173:GLU:HG3	1.89	0.54
5:2:266:ARG:O	5:2:266:ARG:NE	2.40	0.54
14:A6:246:THR:HG23	14:A6:248:GLU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BU:607:CHL:C9	23:BU:607:CHL:C11	2.84	0.54
1:5:86:SER:OG	24:5:602:CLA:O1A	2.23	0.54
1:5:138:ILE:HD13	1:5:158:ILE:HB	1.88	0.54
24:5:613:CLA:C4C	24:5:613:CLA:H51	2.37	0.54
4:b:183:PRO:HB2	4:b:185:TRP:HE1	1.73	0.54
2:0:91:LYS:HZ3	1:AA:83:ALA:CA	2.21	0.54
24:0:610:CLA:H2	25:0:615:LUT:H28	1.88	0.54
1:AA:97:GLU:O	1:AA:101:ILE:HG22	2.06	0.54
3:AB:175:ALA:HA	24:BU:601:CLA:HBB2	1.90	0.54
4:v:294:GLU:HG2	4:v:294:GLU:O	2.08	0.54
23:A6:606:CHL:C9	23:A6:606:CHL:H112	2.37	0.54
23:BJ:609:CHL:HBB1	23:BQ:601:CHL:H52	1.88	0.54
14:BV:80:GLU:OE1	14:BV:80:GLU:N	2.40	0.54
22:BU:209:GLU:OE2	22:BU:211:ASP:N	2.40	0.54
3:8:188:TYR:CD2	3:8:214:TYR:HB3	2.43	0.54
18:X:94:GLY:O	18:X:98:THR:HG23	2.08	0.54
10:i:2:LEU:HD21	17:w:85:MET:HE2	1.88	0.54
20:a:308:ASP:OD1	20:a:312:ARG:N	2.37	0.54
16:A8:82:GLU:OE1	16:A8:82:GLU:N	2.35	0.54
17:A0:92:LEU:HD22	17:A0:97:SER:HA	1.90	0.54
8:BB:103:SER:HB2	8:BB:219:GLY:HA3	1.88	0.54
2:6:240:GLU:HA	2:6:243:LEU:HG	1.90	0.54
8:y:169:MET:HE1	23:y:310:CHL:NC	2.22	0.54
19:z:15:THR:O	19:z:19:LEU:HG	2.07	0.54
19:z:33:TRP:CZ3	19:z:40:VAL:HG11	2.42	0.54
25:9:616:LUT:H181	25:9:616:LUT:C8	2.38	0.54
24:0:603:CLA:HMD2	23:0:609:CHL:H52	1.89	0.54
3:AB:102:GLU:OE2	3:AB:233:ARG:NE	2.31	0.54
5:2:232:THR:H	20:R:269:ARG:HH12	1.54	0.54
23:Au:607:CHL:C10	23:Au:607:CHL:C6	2.85	0.54
17:A0:85:MET:HB3	17:A0:87:THR:HG23	1.90	0.54
18:BA:94:GLY:O	18:BA:98:THR:HG23	2.08	0.54
24:BE:602:CLA:H102	29:BK:101:BCR:H402	1.89	0.54
8:BQ:107:MET:CE	24:BQ:610:CLA:HAB	2.38	0.54
23:Ba:302:CHL:H41	27:Ba:319:LHG:H192	1.90	0.54
4:B:41:GLU:CD	4:B:62:VAL:HG22	2.32	0.54
23:N:609:CHL:C9	23:N:609:CHL:C11	2.85	0.54
8:Y:107:MET:CE	24:Y:311:CLA:HHC	2.38	0.54
23:g:606:CHL:HMC	25:g:616:LUT:H163	1.89	0.54
23:g:609:CHL:HBB1	23:n:601:CHL:H52	1.89	0.54
32:l:102:SQD:H251	32:l:102:SQD:H92	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:76:GLY:HA3	8:n:216:LEU:HD23	1.89	0.54
14:s:220:LEU:O	14:s:224:LYS:HG2	2.08	0.54
24:0:611:CLA:O2D	24:0:611:CLA:H2A	2.08	0.54
24:AA:314:CLA:HBA1	24:AA:314:CLA:HBD	1.89	0.54
32:Az:101:SQD:H92	32:Az:101:SQD:H251	1.90	0.54
5:BG:162:PRO:HB3	5:BG:171:ALA:HB2	1.90	0.54
9:BK:66:LEU:HB3	18:BZ:81:PRO:HG3	1.89	0.54
32:BO:102:SQD:H92	32:BO:102:SQD:H251	1.89	0.54
8:BQ:111:LEU:HA	8:BQ:114:VAL:HG12	1.90	0.54
20:R:201:GLY:HA3	20:R:286:THR:OG1	2.07	0.54
24:1:513:CLA:H92	27:1:521:LHG:H122	1.90	0.54
2:6:162:PHE:CE2	2:6:166:LEU:HD21	2.43	0.54
2:6:209:LEU:HD21	24:6:610:CLA:H3A	1.88	0.54
24:6:611:CLA:O2D	24:6:611:CLA:H2A	2.08	0.54
28:g:619:XAT:H203	24:n:613:CLA:H52	1.90	0.54
14:s:103:LYS:HD3	14:s:106:ASN:ND2	2.22	0.54
14:s:224:LYS:NZ	24:s:611:CLA:O1A	2.41	0.54
16:u:82:GLU:O	16:u:86:LYS:HG2	2.08	0.54
19:z:27:PHE:HB3	21:c:134:LEU:HD23	1.89	0.54
6:3:70:PHE:N	16:A8:103:TYR:OH	2.41	0.54
6:BH:30:LEU:HD11	7:BI:22:VAL:HG13	1.89	0.54
23:BJ:609:CHL:HBC3	23:BJ:609:CHL:HMC	1.90	0.54
24:BJ:610:CLA:H72	25:BJ:615:LUT:H30	1.90	0.54
22:BU:192:ILE:O	22:BU:196:VAL:HG13	2.08	0.54
8:G:103:SER:O	8:G:107:MET:HG3	2.07	0.54
28:G:619:XAT:H15	24:N:613:CLA:H102	1.90	0.54
24:b:602:CLA:H102	29:h:101:BCR:H402	1.89	0.54
8:g:73:GLU:OE2	8:g:73:GLU:N	2.30	0.54
8:g:172:VAL:HA	8:g:175:TYR:HD1	1.73	0.54
14:s:80:GLU:N	14:s:80:GLU:OE1	2.40	0.54
20:a:120:LEU:HB3	24:c:506:CLA:H191	1.90	0.54
1:9:107:MET:HE1	24:9:610:CLA:HAB	1.90	0.54
3:AB:81:PHE:N	24:AB:301:CLA:OBD	2.41	0.54
4:v:263:THR:HG23	4:v:268:PHE:CD2	2.43	0.54
8:A2:103:SER:O	8:A2:107:MET:HG3	2.07	0.54
8:BJ:217:LYS:HZ3	24:BJ:611:CLA:CGD	2.21	0.54
22:BU:250:MET:CE	24:BU:602:CLA:HHC	2.34	0.54
24:BU:602:CLA:H101	28:BU:616:XAT:H28	1.89	0.54
24:BU:604:CLA:HBA1	24:BU:604:CLA:CHA	2.38	0.54
4:b:223:GLN:HB2	4:b:224:ARG:CZ	2.38	0.54
18:x:94:GLY:O	18:x:98:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:176:ILE:HG12	24:A:406:CLA:HED1	1.90	0.54
2:0:163:GLN:HE22	23:0:607:CHL:HMC	1.72	0.54
24:AB:308:CLA:CBB	25:AB:311:LUT:H32	2.37	0.54
22:BU:142:ILE:HG13	23:BU:607:CHL:HED1	1.90	0.54
2:6:156:ILE:O	2:6:160:LEU:HG	2.07	0.54
6:E:70:PHE:N	16:U:103:TYR:OH	2.41	0.54
24:S:610:CLA:HAB	27:C:521:LHG:H101	1.90	0.54
5:d:151:ILE:O	5:d:155:VAL:HG13	2.08	0.54
5:d:153:VAL:O	5:d:157:VAL:HG12	2.08	0.54
8:g:217:LYS:HZ3	24:g:611:CLA:CGD	2.21	0.54
8:n:165:GLN:HG3	23:n:606:CHL:HMA3	1.90	0.54
16:u:83:ALA:HA	16:u:86:LYS:HZ2	1.73	0.54
21:C:81:MET:HG3	21:C:86:LEU:HD12	1.89	0.54
22:r:141:LEU:HD13	22:r:216:LEU:CD1	2.38	0.54
2:0:171:GLU:O	2:0:174:ARG:HB3	2.08	0.54
8:Ba:80:TRP:CD1	8:Ba:82:THR:HG23	2.43	0.54
2:6:48:TYR:HE2	2:6:207:ALA:HB1	1.73	0.53
7:f:17:VAL:HG23	7:f:18:HIS:HD1	1.73	0.53
28:9:619:XAT:H381	28:9:619:XAT:H393	1.90	0.53
14:BV:224:LYS:NZ	24:BV:611:CLA:O1A	2.41	0.53
21:BF:206:PRO:HA	21:BF:209:ILE:HG22	1.89	0.53
24:BF:508:CLA:H2	24:BF:508:CLA:HMA2	1.90	0.53
22:BU:66:ASP:OD2	22:BU:66:ASP:N	2.41	0.53
2:6:157:LEU:HD12	2:6:158:ALA:N	2.23	0.53
4:B:223:GLN:HE22	4:B:224:ARG:NH1	2.06	0.53
24:G:613:CLA:H72	28:Y:301:XAT:H203	1.89	0.53
15:T:6:TYR:O	15:T:10:LEU:HD22	2.08	0.53
19:Z:9:VAL:O	19:Z:13:ILE:HG12	2.07	0.53
27:0:617:LHG:HC91	27:0:617:LHG:H271	1.89	0.53
1:AA:230:PHE:CZ	23:AA:308:CHL:H51	2.44	0.53
24:AA:314:CLA:HMB2	25:AA:316:LUT:H162	1.91	0.53
3:AB:224:LEU:HD13	24:AB:308:CLA:HMA2	1.90	0.53
15:A7:8:PHE:HE1	29:BE:601:BCR:H361	1.74	0.53
14:BV:103:LYS:HD3	14:BV:106:ASN:ND2	2.22	0.53
14:BV:196:PHE:CD2	23:BV:607:CHL:HBC3	2.43	0.53
21:1:318:LEU:HD12	21:1:340:TYR:HB3	1.90	0.53
24:BF:514:CLA:HBD	24:BF:514:CLA:HBA1	1.89	0.53
24:5:604:CLA:HMB2	25:5:616:LUT:H162	1.90	0.53
5:d:159:LEU:O	5:d:163:LEU:HD23	2.08	0.53
23:g:609:CHL:HBC3	23:g:609:CHL:HMC	1.91	0.53
14:s:123:LEU:HG	24:s:604:CLA:CAB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:337:LEU:HB3	21:c:342:MET:SD	2.48	0.53
8:A2:207:ALA:O	8:A2:211:LEU:HG	2.08	0.53
14:A6:160:LEU:HD11	24:A6:604:CLA:HAA1	1.90	0.53
24:A6:610:CLA:HAB	27:1:521:LHG:H101	1.90	0.53
8:BB:76:GLY:HA3	8:BB:216:LEU:HD23	1.90	0.53
8:BQ:88:ASP:OD2	8:BQ:90:GLU:HG3	2.08	0.53
8:BQ:186:ALA:HB2	23:BQ:608:CHL:HBC1	1.89	0.53
22:BU:59:TYR:HD1	22:BU:62:ALA:HB2	1.74	0.53
24:7:313:CLA:HAB	25:7:316:LUT:C15	2.38	0.53
24:B:603:CLA:HAB	24:B:605:CLA:H152	1.89	0.53
21:C:297:TYR:OH	24:C:502:CLA:O1A	2.25	0.53
1:9:158:ILE:O	1:9:161:ILE:HG22	2.08	0.53
1:AA:96:ARG:O	1:AA:100:VAL:HG13	2.09	0.53
24:v:607:CLA:H192	12:Az:28:LEU:HD11	1.90	0.53
5:2:215:HIS:ND1	31:2:404:PL9:O2	2.41	0.53
8:BJ:172:VAL:HA	8:BJ:175:TYR:HD1	1.74	0.53
24:BU:612:CLA:HMB2	25:BU:615:LUT:H162	1.90	0.53
24:6:602:CLA:H72	25:6:616:LUT:H30	1.89	0.53
8:N:105:TRP:CE2	23:N:608:CHL:HED2	2.44	0.53
28:N:619:XAT:H203	24:Y:314:CLA:H52	1.90	0.53
23:S:606:CHL:C9	23:S:606:CHL:C11	2.86	0.53
23:S:606:CHL:C9	23:S:606:CHL:H112	2.38	0.53
8:Y:107:MET:HE1	24:Y:311:CLA:HHC	1.91	0.53
8:Y:110:ALA:CA	8:Y:226:MET:HE1	2.37	0.53
23:g:607:CHL:C10	23:g:607:CHL:C6	2.87	0.53
20:A:183:MET:HE2	24:A:406:CLA:HAC1	1.90	0.53
20:a:92:HIS:ND1	21:c:219:GLY:O	2.40	0.53
1:9:214:LYS:HD3	24:9:612:CLA:HAA2	1.90	0.53
2:0:162:PHE:CZ	2:0:166:LEU:HD11	2.44	0.53
4:v:247:PHE:HE1	24:v:602:CLA:H122	1.73	0.53
28:A2:619:XAT:H203	24:BB:314:CLA:H52	1.90	0.53
7:BI:17:VAL:HG23	7:BI:18:HIS:HD1	1.72	0.53
24:B:601:CLA:HAC1	29:H:101:BCR:H383	1.90	0.53
24:B:605:CLA:H193	24:B:609:CLA:CBB	2.38	0.53
4:b:384:ARG:NH2	5:d:353:LEU:OXT	2.42	0.53
5:d:56:VAL:O	5:d:67:SER:HB3	2.08	0.53
5:d:84:ASN:ND2	5:d:166:SER:OG	2.41	0.53
23:r:605:CHL:HMC	23:r:606:CHL:C3C	2.38	0.53
14:A6:87:GLY:HA2	14:A6:92:ASP:OD1	2.09	0.53
20:BD:20:TRP:HE1	32:BD:412:SQD:HO3	1.52	0.53
4:B:263:THR:HG23	4:B:268:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:350:GLY:HA2	20:A:334:ARG:HG3	1.89	0.53
9:h:52:VAL:O	9:h:56:ILE:HG12	2.09	0.53
8:n:186:ALA:HB2	23:n:608:CHL:HBC1	1.90	0.53
23:y:302:CHL:C9	23:y:302:CHL:H112	2.39	0.53
1:9:196:PHE:O	25:9:615:LUT:H24	2.09	0.53
14:A6:135:ASN:OD1	14:A6:145:ALA:HB3	2.09	0.53
8:BB:219:GLY:O	8:BB:223:MET:HG3	2.08	0.53
8:BQ:239:GLY:O	8:BQ:243:ASN:ND2	2.42	0.53
14:BV:229:GLY:O	14:BV:233:MET:HG2	2.08	0.53
21:1:45:LEU:HD12	21:1:138:GLU:HB3	1.90	0.53
20:BD:120:LEU:HB3	24:BF:506:CLA:H191	1.90	0.53
24:BD:405:CLA:C2	38:BD:408:PHO:HBB1	2.39	0.53
8:N:113:CYS:HG	8:N:131:TRP:CG	2.26	0.53
8:N:207:ALA:O	8:N:211:LEU:HG	2.09	0.53
21:c:164:HIS:O	21:c:168:LEU:HG	2.09	0.53
24:c:505:CLA:HBC2	24:c:505:CLA:HHD	1.91	0.53
24:r:602:CLA:H3A	24:r:602:CLA:CGA	2.38	0.53
23:0:607:CHL:HBB2	23:0:609:CHL:HBC1	1.90	0.53
8:A2:105:TRP:CE2	23:A2:608:CHL:HED2	2.44	0.53
23:5:601:CHL:HHD	23:5:601:CHL:HBC2	1.91	0.53
24:g:610:CLA:H72	25:g:615:LUT:H30	1.90	0.53
8:y:80:TRP:CD1	8:y:82:THR:HG23	2.44	0.53
2:0:209:LEU:HG	24:0:610:CLA:CMA	2.39	0.53
8:BQ:76:GLY:HA3	8:BQ:216:LEU:HD23	1.90	0.53
9:H:48:ALA:O	9:H:52:VAL:HG22	2.08	0.53
8:Y:187:GLU:N	8:Y:187:GLU:OE2	2.42	0.53
8:n:220:ARG:HB3	27:n:618:LHG:H252	1.90	0.53
24:C:505:CLA:H11	34:C:517:DGD:HB42	1.91	0.53
21:c:42:LEU:HD21	24:c:512:CLA:H2A	1.90	0.53
22:r:209:GLU:OE2	22:r:215:ARG:HG2	2.08	0.53
4:v:30:VAL:HG12	24:v:605:CLA:HHD	1.91	0.53
5:2:183:ILE:HG23	24:2:402:CLA:HAC1	1.91	0.53
23:A6:606:CHL:C9	23:A6:606:CHL:C11	2.86	0.53
21:BF:337:LEU:HB3	21:BF:342:MET:SD	2.48	0.53
24:7:314:CLA:HBD	24:7:314:CLA:HBA1	1.90	0.52
3:8:188:TYR:HD2	3:8:214:TYR:HB3	1.74	0.52
4:B:60:MET:HA	4:B:60:MET:HE3	1.92	0.52
24:S:602:CLA:H61	25:S:615:LUT:H373	1.92	0.52
8:g:231:VAL:HG11	24:g:613:CLA:HAC2	1.91	0.52
11:k:41:PRO:HB3	21:c:67:MET:HE2	1.91	0.52
23:n:606:CHL:HBB2	23:n:607:CHL:CBB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:201:ASN:OD1	21:C:201:ASN:N	2.40	0.52
20:a:61:ASP:HB3	20:a:63:ILE:HG12	1.91	0.52
21:c:39:ASN:HB2	24:c:509:CLA:HBA1	1.91	0.52
2:0:77:TRP:HD1	2:0:79:THR:HG23	1.73	0.52
3:AB:162:VAL:O	3:AB:166:ASN:N	2.42	0.52
24:v:601:CLA:HAC1	29:Av:101:BCR:H383	1.91	0.52
5:BG:265:LYS:HZ2	20:BD:246:TYR:HD1	1.53	0.52
2:6:77:TRP:HD1	2:6:79:THR:HG23	1.73	0.52
4:B:30:VAL:HG12	24:B:605:CLA:HHD	1.91	0.52
24:B:614:CLA:H11	24:B:614:CLA:CHA	2.39	0.52
27:D:404:LHG:H282	27:D:404:LHG:H122	1.90	0.52
6:E:27:ILE:HB	6:E:28:PRO:HD3	1.92	0.52
14:s:113:PHE:HD1	24:s:608:CLA:HED1	1.73	0.52
20:A:184:ILE:HG23	20:A:328:MET:HE3	1.91	0.52
24:a:405:CLA:C2	38:a:408:PHO:HBB1	2.39	0.52
21:c:82:TYR:HE1	21:c:398:HIS:HD2	1.56	0.52
22:r:126:PRO:HG2	22:r:127:TYR:CD1	2.44	0.52
24:9:602:CLA:HAB	25:9:616:LUT:C32	2.38	0.52
24:AB:308:CLA:CAB	25:AB:311:LUT:H32	2.39	0.52
19:BC:9:VAL:O	19:BC:13:ILE:HG12	2.09	0.52
8:BJ:165:GLN:O	8:BJ:169:MET:HG3	2.09	0.52
14:BV:113:PHE:HD1	24:BV:608:CLA:HED1	1.74	0.52
14:BV:230:ARG:HA	14:BV:233:MET:HE2	1.90	0.52
8:Ba:114:VAL:HG22	8:Ba:118:LEU:HD11	1.91	0.52
1:5:90:GLU:O	1:5:94:ARG:HG2	2.09	0.52
1:5:238:LYS:HD2	1:5:242:GLU:OE2	2.09	0.52
8:N:206:GLU:OE1	8:N:206:GLU:N	2.30	0.52
8:g:165:GLN:O	8:g:169:MET:HG3	2.09	0.52
22:r:194:ILE:O	22:r:198:VAL:HG22	2.09	0.52
1:9:90:GLU:O	1:9:94:ARG:HG2	2.09	0.52
2:0:157:LEU:H	2:0:157:LEU:HD12	1.74	0.52
24:v:605:CLA:HBB1	24:v:606:CLA:H51	1.91	0.52
24:v:614:CLA:H11	24:v:614:CLA:CHA	2.39	0.52
8:BJ:183:LEU:HG	23:BJ:608:CHL:HBB1	1.90	0.52
21:1:201:ASN:OD1	21:1:201:ASN:N	2.40	0.52
22:BU:59:TYR:CD1	22:BU:62:ALA:HB2	2.44	0.52
2:6:45:ASP:N	2:6:45:ASP:OD1	2.42	0.52
23:6:601:CHL:C9	23:6:601:CHL:C6	2.88	0.52
8:y:60:GLY:HA3	23:y:302:CHL:HBB1	1.89	0.52
8:y:89:PRO:HD2	8:y:90:GLU:N	2.20	0.52
21:c:318:LEU:HD12	21:c:340:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:242:LEU:HD22	25:0:615:LUT:H172	1.90	0.52
1:AA:103:SER:HB2	1:AA:219:GLY:HA3	1.92	0.52
24:BE:610:CLA:CHC	29:BK:101:BCR:HC8	2.38	0.52
14:BV:220:LEU:O	14:BV:224:LYS:HG2	2.09	0.52
20:R:20:TRP:HE1	32:R:411:SQD:HO3	1.56	0.52
20:R:184:ILE:HG23	20:R:328:MET:CE	2.33	0.52
5:D:266:ARG:C	5:D:266:ARG:HE	2.16	0.52
22:r:191:LEU:O	22:r:195:GLU:HG2	2.10	0.52
2:0:77:TRP:CD1	2:0:79:THR:HG23	2.45	0.52
24:AA:311:CLA:O2A	25:AA:316:LUT:O23	2.27	0.52
8:A2:227:PHE:HE1	23:A2:609:CHL:H203	1.74	0.52
8:A2:228:GLY:O	8:A2:232:GLN:HG3	2.09	0.52
23:BJ:606:CHL:HAA1	23:BJ:606:CHL:CGD	2.40	0.52
8:BQ:106:ALA:HA	8:BQ:226:MET:HE1	1.92	0.52
21:BF:78:GLU:HB2	21:BF:79:LYS:HZ2	1.74	0.52
24:BU:602:CLA:H3A	24:BU:602:CLA:CGA	2.39	0.52
2:6:77:TRP:CD1	2:6:79:THR:HG23	2.45	0.52
2:6:234:THR:HG23	2:6:236:LYS:H	1.74	0.52
4:B:25:MET:HE1	4:B:108:PHE:HD1	1.74	0.52
5:D:202:VAL:HG22	24:D:401:CLA:C2B	2.40	0.52
8:Y:76:GLY:HA3	8:Y:216:LEU:HD23	1.91	0.52
20:a:20:TRP:HE1	32:a:412:SQD:HO3	1.54	0.52
2:0:102:TRP:CD1	23:0:609:CHL:HMD3	2.44	0.52
24:AA:304:CLA:OBD	23:AA:310:CHL:H2	2.10	0.52
3:AB:99:ARG:NH2	3:AB:102:GLU:OE1	2.42	0.52
5:2:202:VAL:HG22	24:2:402:CLA:C2B	2.39	0.52
8:Au:188:ASP:OD2	8:Au:191:TYR:N	2.38	0.52
4:BE:203:ILE:O	4:BE:207:THR:HG23	2.10	0.52
8:N:141:ASP:OD1	8:N:142:GLY:N	2.43	0.52
8:N:220:ARG:HD3	24:N:602:CLA:CHD	2.40	0.52
25:N:616:LUT:H181	25:N:616:LUT:C8	2.40	0.52
4:b:256:MET:HA	4:b:256:MET:HE2	1.92	0.52
8:n:239:GLY:O	8:n:243:ASN:ND2	2.42	0.52
21:c:396:MET:SD	21:c:397:THR:HG23	2.50	0.52
22:r:142:ILE:HG13	23:r:607:CHL:HED1	1.91	0.52
22:r:223:PHE:O	25:r:615:LUT:H24	2.09	0.52
2:0:208:GLU:O	2:0:212:LYS:HG2	2.09	0.52
8:BB:187:GLU:N	8:BB:187:GLU:OE2	2.43	0.52
14:BV:209:LEU:HD12	25:BV:614:LUT:H222	1.92	0.52
22:BU:190:THR:O	22:BU:194:ILE:HG12	2.10	0.52
24:6:610:CLA:HMB2	24:6:612:CLA:HBA2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:314:CLA:HMB2	25:7:316:LUT:H162	1.92	0.52
14:s:196:PHE:CD2	23:s:607:CHL:HBC3	2.44	0.52
15:t:3:ALA:O	15:t:7:THR:HG23	2.09	0.52
1:9:161:ILE:HD11	23:9:606:CHL:C2D	2.40	0.52
2:0:209:LEU:HD21	24:0:610:CLA:O1A	2.09	0.52
5:2:350:GLY:HA2	20:R:334:ARG:HG3	1.91	0.52
24:A2:614:CLA:HBD	24:A2:614:CLA:HBA1	1.91	0.52
24:BE:610:CLA:C3B	29:BK:101:BCR:H323	2.40	0.52
21:BF:318:LEU:HD12	21:BF:340:TYR:HB3	1.92	0.52
4:B:25:MET:HE1	4:B:108:PHE:CD1	2.45	0.52
14:S:196:PHE:CD2	23:S:607:CHL:HBC3	2.45	0.52
8:Y:152:LEU:O	8:Y:154:HIS:N	2.42	0.52
4:b:203:ILE:O	4:b:207:THR:HG23	2.10	0.52
20:a:176:ILE:HG12	24:a:406:CLA:HED1	1.91	0.52
23:0:601:CHL:C9	23:0:601:CHL:C6	2.88	0.52
1:AA:94:ARG:NH1	1:AA:94:ARG:HB2	2.25	0.52
4:v:226:TYR:HA	4:v:231:MET:SD	2.50	0.52
4:v:472:ARG:HD3	4:v:479:PHE:CZ	2.45	0.52
8:Au:136:SER:HB3	23:Au:607:CHL:HED2	1.92	0.52
8:A2:141:ASP:OD1	8:A2:142:GLY:N	2.43	0.52
6:BH:35:TRP:CD2	7:BI:33:ALA:HB2	2.45	0.52
24:BU:609:CLA:H2	25:BU:615:LUT:H26	1.92	0.52
1:5:165:GLN:HE22	23:5:606:CHL:C1A	2.23	0.52
1:5:214:LYS:HD3	24:5:612:CLA:HAA2	1.91	0.52
25:5:615:LUT:H181	25:5:615:LUT:C8	2.39	0.52
24:B:605:CLA:H193	24:B:609:CLA:HBB2	1.92	0.52
23:N:605:CHL:HMB2	14:S:137:TYR:OH	2.10	0.52
24:N:610:CLA:H62	24:N:612:CLA:HBA1	1.92	0.52
23:g:606:CHL:HAA1	23:g:606:CHL:CGD	2.40	0.52
22:r:250:MET:CE	24:r:602:CLA:HHC	2.34	0.52
25:9:615:LUT:H181	25:9:615:LUT:C8	2.40	0.52
8:BQ:211:LEU:CD1	24:BQ:610:CLA:H3A	2.40	0.52
8:Ba:161:ILE:HD11	23:Ba:307:CHL:C1D	2.39	0.52
3:8:81:PHE:N	24:8:301:CLA:OBD	2.39	0.51
5:D:344:GLU:OE2	5:D:349:ARG:NH1	2.43	0.51
7:f:13:ARG:O	7:f:17:VAL:HG22	2.10	0.51
8:g:183:LEU:HG	23:g:608:CHL:HBB1	1.91	0.51
24:y:305:CLA:HBA1	23:y:307:CHL:CHD	2.40	0.51
1:9:56:VAL:HG21	23:9:601:CHL:HBC3	1.92	0.51
2:0:172:GLY:HA3	1:AA:62:PHE:CZ	2.42	0.51
2:0:197:LEU:HD13	25:0:615:LUT:H222	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:169:MET:HA	1:AA:172:VAL:HG22	1.92	0.51
3:AB:146:LEU:O	3:AB:150:LEU:HG	2.11	0.51
24:v:607:CLA:HAC2	29:v:622:BCR:H272	1.92	0.51
13:A1:18:PRO:O	13:A1:22:LEU:HG	2.09	0.51
8:A2:58:TYR:CE2	8:A2:59:LEU:HD21	2.45	0.51
14:A6:207:ASP:OD1	25:A6:614:LUT:O23	2.28	0.51
8:BB:90:GLU:OE1	8:BB:90:GLU:N	2.35	0.51
8:BB:231:VAL:HG11	24:BB:314:CLA:HAC2	1.92	0.51
8:BQ:217:LYS:NZ	27:BQ:618:LHG:O4	2.38	0.51
21:BF:102:GLY:N	21:BF:194:GLY:O	2.42	0.51
22:BU:126:PRO:HG2	22:BU:127:TYR:CD1	2.44	0.51
2:6:194:PHE:O	25:6:615:LUT:H24	2.10	0.51
5:D:183:ILE:HG23	24:D:401:CLA:HAC1	1.91	0.51
8:G:188:ASP:OD2	8:G:191:TYR:N	2.39	0.51
24:N:614:CLA:HBD	24:N:614:CLA:HBA1	1.93	0.51
5:d:121:PHE:HA	5:d:124:ILE:HG22	1.91	0.51
15:t:10:LEU:O	15:t:14:LEU:HD23	2.11	0.51
21:C:180:LEU:HD11	21:C:202:LEU:HD21	1.92	0.51
1:9:125:LYS:HZ1	1:9:148:GLY:HA3	1.75	0.51
3:AB:239:MET:CE	3:AB:243:TYR:HB2	2.40	0.51
8:BJ:247:HIS:CG	24:BJ:613:CLA:HAA2	2.45	0.51
23:BJ:607:CHL:C10	23:BJ:607:CHL:C6	2.87	0.51
22:BU:147:ALA:HB2	28:BU:616:XAT:H202	1.91	0.51
22:BU:223:PHE:O	25:BU:615:LUT:H24	2.10	0.51
2:6:226:GLY:O	2:6:230:GLN:NE2	2.44	0.51
24:7:304:CLA:OBD	23:7:310:CHL:H2	2.10	0.51
3:8:239:MET:CE	3:8:243:TYR:HB2	2.40	0.51
14:S:110:TYR:HD1	24:S:602:CLA:H12	1.74	0.51
24:Y:311:CLA:CHB	24:Y:311:CLA:H2	2.41	0.51
8:y:97:GLU:O	8:y:101:ILE:HG22	2.09	0.51
8:y:246:ASP:OD1	8:y:254:ASN:HB3	2.10	0.51
21:C:215:LYS:NZ	21:C:226:SER:OG	2.33	0.51
2:0:45:ASP:N	2:0:45:ASP:OD1	2.42	0.51
1:AA:214:LYS:HE2	24:AA:313:CLA:HBD	1.91	0.51
34:1:517:DGD:HB31	30:1:519:LMG:H321	1.93	0.51
3:8:108:TRP:CD1	23:8:307:CHL:HMD3	2.46	0.51
24:8:308:CLA:CGA	24:8:308:CLA:H3A	2.37	0.51
24:B:615:CLA:H72	29:B:619:BCR:H353	1.93	0.51
5:D:22:TRP:HA	5:D:25:ARG:HH21	1.75	0.51
8:G:196:PHE:O	25:G:615:LUT:H24	2.11	0.51
24:G:612:CLA:HMC3	25:G:615:LUT:H191	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:201:LEU:HD12	24:N:610:CLA:H11	1.92	0.51
27:b:624:LHG:H172	12:l:20:TRP:HZ3	1.76	0.51
3:AB:153:MET:HE2	3:AB:157:GLU:CD	2.36	0.51
9:Av:18:THR:HA	9:Av:21:LYS:HE3	1.92	0.51
8:BB:152:LEU:O	8:BB:154:HIS:N	2.41	0.51
5:BG:71:GLY:HA3	7:BI:39:ARG:HH22	1.76	0.51
7:BI:13:ARG:O	7:BI:17:VAL:HG22	2.11	0.51
8:Ba:60:GLY:HA3	23:Ba:302:CHL:HBB1	1.91	0.51
19:Bb:33:TRP:CZ3	19:Bb:40:VAL:HG21	2.45	0.51
20:BD:176:ILE:HG12	24:BD:406:CLA:HED1	1.93	0.51
1:7:96:ARG:O	1:7:100:VAL:HG13	2.09	0.51
1:7:236:THR:HG23	1:7:238:LYS:H	1.75	0.51
3:8:204:GLY:HA3	3:8:208:LYS:HE3	1.92	0.51
5:D:321:LEU:HB3	20:A:331:MET:HE1	1.91	0.51
8:N:169:MET:HA	8:N:172:VAL:HG22	1.92	0.51
24:b:612:CLA:CED	24:b:612:CLA:H2A	2.40	0.51
20:A:289:GLY:O	20:A:293:MET:HG2	2.11	0.51
21:C:26:ARG:CZ	24:C:511:CLA:CAD	2.88	0.51
20:a:199:MET:O	20:a:202:VAL:HG12	2.11	0.51
22:r:147:ALA:HB2	28:r:616:XAT:H202	1.92	0.51
9:Av:48:ALA:O	9:Av:52:VAL:HG22	2.09	0.51
8:A2:206:GLU:CD	8:A2:206:GLU:H	2.18	0.51
14:A6:229:GLY:O	14:A6:233:MET:HG3	2.11	0.51
23:BB:302:CHL:HBB1	23:BB:302:CHL:HHC	1.91	0.51
5:BG:242:GLU:HG3	20:BD:242:GLU:OE1	2.09	0.51
14:BV:112:ALA:HA	14:BV:200:LEU:HD11	1.91	0.51
17:W:131:LEU:CD2	21:C:452:ALA:HB1	2.41	0.51
8:Y:231:VAL:HG11	24:Y:314:CLA:HAC2	1.93	0.51
4:b:224:ARG:HH21	4:b:227:LYS:NZ	2.09	0.51
5:d:351:ASN:ND2	20:a:336:ALA:O	2.44	0.51
13:m:13:LEU:O	13:m:17:VAL:HG23	2.10	0.51
1:AA:236:THR:HG23	1:AA:238:LYS:H	1.76	0.51
3:AB:201:ASP:OD1	24:AB:308:CLA:HAA1	2.11	0.51
3:AB:203:LEU:HD23	25:AB:311:LUT:H222	1.93	0.51
24:BE:610:CLA:C3D	9:BK:43:MET:HE1	2.41	0.51
5:BG:265:LYS:NZ	20:BD:246:TYR:HE1	2.08	0.51
23:BQ:606:CHL:HBB2	23:BQ:607:CHL:CBB	2.40	0.51
14:BV:239:PHE:CE1	25:BV:614:LUT:H41	2.45	0.51
24:G:611:CLA:H51	24:G:612:CLA:C3D	2.41	0.51
14:S:217:GLN:OE1	14:S:217:GLN:N	2.44	0.51
5:d:71:GLY:HA3	7:f:39:ARG:HH22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:s:239:PHE:CE1	25:s:614:LUT:H41	2.46	0.51
24:c:508:CLA:HMA2	24:c:508:CLA:H2	1.93	0.51
3:AB:187:ASN:ND2	3:AB:195:PRO:HA	2.25	0.51
3:AB:222:GLU:OE1	3:AB:222:GLU:N	2.31	0.51
5:BG:156:SER:HA	5:BG:160:ILE:CG1	2.40	0.51
22:BU:146:TRP:CE2	24:BU:608:CLA:HBC3	2.46	0.51
24:6:612:CLA:HMC3	25:6:615:LUT:H191	1.91	0.51
22:r:146:TRP:CE2	24:r:608:CLA:HBC3	2.46	0.51
24:r:604:CLA:HBA1	24:r:604:CLA:CHA	2.40	0.51
3:AB:140:PHE:HE1	22:BU:279:LEU:HD13	1.74	0.51
3:AB:150:LEU:HD22	23:AB:307:CHL:HBB2	1.92	0.51
4:BE:256:MET:HE2	4:BE:256:MET:HA	1.91	0.51
4:BE:348:ASN:OD1	4:BE:352:ARG:N	2.44	0.51
11:BN:28:GLU:H	11:BN:28:GLU:CD	2.19	0.51
14:BV:246:THR:HG23	14:BV:248:GLU:H	1.76	0.51
19:Bb:42:SER:O	19:Bb:46:LEU:HG	2.11	0.51
24:5:602:CLA:H12	24:5:602:CLA:H3A	1.93	0.51
4:B:384:ARG:HD3	5:D:353:LEU:HD13	1.91	0.51
8:N:231:VAL:HG21	24:N:613:CLA:CAC	2.39	0.51
19:Z:50:LEU:HA	19:Z:53:LEU:HD12	1.92	0.51
4:b:201:HIS:HB2	24:b:603:CLA:CHB	2.41	0.51
21:C:42:LEU:HD21	24:C:511:CLA:HED1	1.92	0.51
21:C:327:ASN:OD1	21:C:330:SER:OG	2.22	0.51
22:r:59:TYR:HB3	22:r:62:ALA:HB2	1.93	0.51
22:r:166:GLN:OE1	22:r:166:GLN:N	2.34	0.51
22:r:190:THR:O	22:r:194:ILE:HG12	2.11	0.51
3:AB:157:GLU:HG2	3:AB:160:ARG:NH1	2.26	0.51
6:3:27:ILE:HB	6:3:28:PRO:HD3	1.93	0.51
29:Ay:102:BCR:H323	21:1:116:VAL:HG23	1.93	0.51
24:A2:610:CLA:H62	24:A2:612:CLA:HBA1	1.91	0.51
5:BG:121:PHE:HA	5:BG:124:ILE:HG22	1.92	0.51
8:BQ:107:MET:HE3	24:BQ:610:CLA:HAB	1.93	0.51
14:BV:57:ASP:OD1	14:BV:58:GLU:N	2.44	0.51
20:R:176:ILE:HG12	24:R:405:CLA:HED1	1.93	0.51
20:BD:183:MET:HE2	24:BD:406:CLA:HAC1	1.93	0.51
21:BF:78:GLU:HB2	21:BF:79:LYS:NZ	2.25	0.51
1:5:163:ALA:O	1:5:166:VAL:HG22	2.11	0.51
3:8:187:ASN:ND2	3:8:195:PRO:HA	2.26	0.51
28:N:619:XAT:H14	27:Y:319:LHG:H191	1.93	0.51
4:b:468:TRP:NE1	4:b:472:ARG:HH21	2.09	0.51
28:n:619:XAT:H14	27:y:319:LHG:H191	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:s:112:ALA:HA	14:s:200:LEU:HD11	1.91	0.51
24:C:504:CLA:H172	24:C:510:CLA:HBB2	1.93	0.51
21:c:65:GLY:O	21:c:69:LEU:HD23	2.11	0.51
24:r:604:CLA:H12	26:r:617:NEX:H382	1.93	0.51
1:AA:75:PRO:HD2	1:AA:96:ARG:HH22	1.76	0.51
7:4:13:ARG:O	7:4:17:VAL:HG22	2.11	0.51
8:Au:169:MET:HA	8:Au:169:MET:HE2	1.93	0.51
4:BE:169:SER:OG	4:BE:266:GLU:OE1	2.27	0.51
24:BJ:611:CLA:H2	24:BJ:612:CLA:HED3	1.93	0.51
8:Ba:226:MET:HE3	8:Ba:226:MET:O	2.11	0.51
20:R:134:SER:HA	20:R:139:MET:HE2	1.92	0.51
1:5:56:VAL:HG21	23:5:601:CHL:HBC3	1.94	0.50
1:7:157:SER:O	1:7:161:ILE:HD12	2.11	0.50
24:B:609:CLA:C3D	9:H:43:MET:HE1	2.39	0.50
8:G:136:SER:HB3	23:G:607:CHL:HED2	1.93	0.50
14:S:135:ASN:OD1	14:S:145:ALA:HB3	2.10	0.50
14:S:207:ASP:OD1	25:S:614:LUT:O23	2.28	0.50
17:W:85:MET:HB3	17:W:87:THR:HG23	1.92	0.50
17:W:110:GLY:HA3	27:W:201:LHG:H181	1.94	0.50
8:g:247:HIS:CG	24:g:613:CLA:HAA2	2.47	0.50
23:n:601:CHL:HED3	24:n:602:CLA:HBC2	1.93	0.50
23:AA:310:CHL:HHC	23:AA:310:CHL:HBB1	1.93	0.50
8:Ba:246:ASP:OD1	8:Ba:254:ASN:HB3	2.11	0.50
2:6:162:PHE:CZ	2:6:166:LEU:HD11	2.46	0.50
1:7:94:ARG:HB2	1:7:94:ARG:NH1	2.26	0.50
4:b:66:MET:HE2	24:b:606:CLA:HED3	1.93	0.50
4:b:348:ASN:OD1	4:b:352:ARG:N	2.45	0.50
24:b:610:CLA:CHC	29:h:101:BCR:HC8	2.42	0.50
14:s:154:LEU:HD21	14:s:171:LEU:HA	1.93	0.50
14:s:239:PHE:HE1	25:s:614:LUT:H41	1.75	0.50
24:s:604:CLA:C1C	26:s:616:NEX:H222	2.41	0.50
19:z:33:TRP:HZ3	19:z:40:VAL:HG11	1.76	0.50
20:a:283:ILE:HA	20:a:286:THR:HG22	1.92	0.50
1:9:247:HIS:HB2	24:9:613:CLA:HAA2	1.93	0.50
24:0:612:CLA:HMC3	25:0:615:LUT:H191	1.94	0.50
25:0:615:LUT:H181	25:0:615:LUT:C8	2.42	0.50
25:A2:616:LUT:C8	25:A2:616:LUT:H181	2.40	0.50
8:BB:186:ALA:HB2	23:BB:309:CHL:HBC1	1.93	0.50
5:BG:30:PHE:HZ	5:BG:132:GLU:OE2	1.94	0.50
8:BQ:220:ARG:HB3	27:BQ:618:LHG:H252	1.93	0.50
24:1:505:CLA:H11	34:1:517:DGD:HB42	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:603:CLA:HMD2	23:6:609:CHL:H52	1.92	0.50
4:b:223:GLN:H	4:b:223:GLN:CD	2.20	0.50
5:d:152:ALA:O	5:d:156:SER:OG	2.29	0.50
5:2:22:TRP:HA	5:2:25:ARG:HH21	1.76	0.50
8:Au:149:ASN:HB3	8:Au:152:LEU:HG	1.92	0.50
8:Au:196:PHE:O	25:Au:615:LUT:H24	2.11	0.50
19:BC:15:THR:HA	19:BC:18:ILE:HG22	1.93	0.50
5:BG:160:ILE:CD1	5:BG:288:VAL:HG22	2.41	0.50
23:BJ:601:CHL:C10	23:BJ:601:CHL:H61	2.40	0.50
14:BV:154:LEU:HD21	14:BV:171:LEU:HA	1.92	0.50
21:1:215:LYS:NZ	21:1:226:SER:OG	2.34	0.50
21:1:240:LEU:HD21	24:1:502:CLA:CAB	2.41	0.50
21:1:342:MET:HE3	21:1:343:ARG:H	1.75	0.50
21:BF:269:GLU:OE2	21:BF:444:HIS:ND1	2.36	0.50
22:BU:231:ASP:HB3	22:BU:234:LYS:HE3	1.93	0.50
1:7:232:GLN:O	1:7:236:THR:HG22	2.12	0.50
8:G:105:TRP:CD1	23:G:609:CHL:HMD3	2.47	0.50
4:b:201:HIS:HB2	24:b:603:CLA:C1B	2.41	0.50
4:b:226:TYR:CE2	4:b:231:MET:HB2	2.46	0.50
4:b:468:TRP:HE1	4:b:472:ARG:HH21	1.60	0.50
23:g:601:CHL:C10	23:g:601:CHL:H61	2.41	0.50
8:n:95:ASN:HD21	24:n:602:CLA:H12	1.76	0.50
8:n:106:ALA:HA	8:n:226:MET:HE1	1.92	0.50
8:y:113:CYS:HG	8:y:131:TRP:CG	2.29	0.50
21:C:240:LEU:HD21	24:C:502:CLA:CAB	2.40	0.50
21:c:134:LEU:HG	21:c:135:LEU:HD23	1.93	0.50
1:9:86:SER:OG	24:9:602:CLA:O1A	2.25	0.50
1:AA:202:ALA:HB2	24:AA:311:CLA:HAA2	1.93	0.50
14:A6:132:GLU:HG2	14:A6:251:VAL:HB	1.93	0.50
17:A0:98:ASN:OD1	17:A0:100:LEU:HD12	2.11	0.50
4:BE:384:ARG:NH2	5:BG:353:LEU:OXT	2.43	0.50
27:BG:404:LHG:H321	15:BW:21:ILE:HD11	1.93	0.50
8:BJ:176:ARG:NH2	23:BJ:609:CHL:O1D	2.34	0.50
24:BJ:613:CLA:H91	27:BJ:618:LHG:H321	1.92	0.50
24:BV:604:CLA:C1C	26:BV:616:NEX:H222	2.41	0.50
21:BF:104:GLU:OE1	21:BF:104:GLU:N	2.39	0.50
2:6:221:MET:HE1	24:6:602:CLA:CAB	2.41	0.50
24:6:613:CLA:CMB	25:6:615:LUT:H162	2.41	0.50
4:B:242:ILE:HA	4:B:245:VAL:HG12	1.91	0.50
9:H:62:ASN:HA	34:H:102:DGD:HG2	1.93	0.50
27:b:624:LHG:H201	31:d:403:PL9:H311	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:150:PRO:HA	5:d:153:VAL:CG1	2.40	0.50
23:y:307:CHL:OMC	25:y:317:LUT:H163	2.12	0.50
29:z:102:BCR:H323	21:c:116:VAL:HG23	1.93	0.50
24:C:513:CLA:H92	27:C:521:LHG:H122	1.92	0.50
22:r:125:GLN:HB2	24:r:614:CLA:O1D	2.12	0.50
3:AB:78:PRO:HG3	3:AB:225:LYS:HD3	1.93	0.50
4:v:348:ASN:OD1	4:v:352:ARG:N	2.45	0.50
28:A2:619:XAT:H14	27:BB:319:LHG:H191	1.93	0.50
14:A6:188:TYR:O	23:A6:607:CHL:HMC	2.10	0.50
24:BB:303:CLA:HAB	25:BB:317:LUT:H32	1.94	0.50
4:BE:201:HIS:HB2	24:BE:603:CLA:CHB	2.41	0.50
4:BE:210:ILE:O	4:BE:214:LEU:HD12	2.12	0.50
13:BP:25:ILE:O	13:BP:29:THR:HG23	2.12	0.50
20:BD:325:ASN:HA	20:BD:328:MET:HE3	1.92	0.50
1:5:107:MET:HE3	25:5:615:LUT:H34	1.93	0.50
1:5:155:ALA:HA	23:5:605:CHL:CHC	2.42	0.50
1:7:214:LYS:HE2	24:7:313:CLA:HBD	1.93	0.50
7:F:13:ARG:O	7:F:17:VAL:HG22	2.11	0.50
5:d:160:ILE:CD1	5:d:288:VAL:HG22	2.41	0.50
6:e:57:THR:O	6:e:61:GLN:NE2	2.44	0.50
14:s:236:MET:HG3	25:s:615:LUT:H14	1.93	0.50
24:AB:301:CLA:CBB	28:AB:312:XAT:H32	2.42	0.50
4:v:92:SER:OG	4:v:94:GLU:OE1	2.22	0.50
8:BB:252:VAL:O	8:BB:255:ASN:ND2	2.44	0.50
23:BJ:607:CHL:H191	23:BQ:601:CHL:H41	1.94	0.50
1:7:59:LEU:HB2	1:7:63:SER:HA	1.93	0.50
3:8:225:LYS:O	3:8:229:ILE:HG22	2.11	0.50
4:B:121:GLU:HG2	9:H:24:LYS:CE	2.42	0.50
8:G:101:ILE:HG22	23:G:609:CHL:HMD1	1.92	0.50
8:G:182:PRO:HG2	26:G:617:NEX:H192	1.94	0.50
25:N:616:LUT:H181	25:N:616:LUT:H8	1.93	0.50
8:Y:81:ASP:OD1	8:Y:86:SER:OG	2.30	0.50
24:Y:303:CLA:HAB	25:Y:317:LUT:H32	1.94	0.50
11:k:28:GLU:H	11:k:28:GLU:CD	2.20	0.50
23:n:608:CHL:HAB	26:n:617:NEX:H202	1.93	0.50
20:a:104:GLU:OE2	20:a:108:ASN:ND2	2.45	0.50
20:a:140:ARG:HB3	20:a:142:TRP:CZ3	2.47	0.50
21:c:102:GLY:N	21:c:194:GLY:O	2.40	0.50
23:9:601:CHL:HBC2	23:9:601:CHL:HHD	1.92	0.50
2:0:142:LEU:HD21	24:0:604:CLA:HAA2	1.94	0.50
2:0:194:PHE:O	25:0:615:LUT:H24	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:41:GLU:CD	4:v:62:VAL:HG22	2.36	0.50
8:Au:90:GLU:OE2	8:Au:90:GLU:N	2.32	0.50
9:Av:65:VAL:HG23	9:Av:67:LEU:HB3	1.94	0.50
4:BE:170:ASP:OD2	4:BE:175:THR:N	2.44	0.50
6:BH:57:THR:O	6:BH:61:GLN:NE2	2.45	0.50
23:BQ:609:CHL:C9	23:BQ:609:CHL:H112	2.42	0.50
1:7:239:GLY:O	1:7:243:ASN:ND2	2.39	0.50
24:7:311:CLA:O2A	25:7:316:LUT:O23	2.28	0.50
12:l:22:LEU:HB3	15:t:16:ILE:HD13	1.92	0.50
18:x:97:LEU:O	18:x:101:ILE:HG12	2.12	0.50
19:z:1:MET:CE	2:0:149:ASN:HB3	2.42	0.50
20:A:287:ALA:HA	20:A:290:ILE:HG22	1.93	0.50
24:C:512:CLA:H161	24:C:513:CLA:H13	1.94	0.50
3:AB:224:LEU:CD1	24:AB:308:CLA:HMA2	2.41	0.50
4:v:122:ILE:HA	9:Av:24:LYS:HZ3	1.77	0.50
4:v:384:ARG:HB2	5:2:353:LEU:HD22	1.93	0.50
24:v:604:CLA:H172	27:v:621:LHG:H311	1.94	0.50
8:A2:231:VAL:HG21	24:A2:613:CLA:CAC	2.39	0.50
20:BD:201:GLY:HA3	20:BD:286:THR:OG1	2.11	0.50
1:5:247:HIS:HB2	24:5:613:CLA:HAA2	1.94	0.50
8:G:107:MET:HE1	24:G:610:CLA:HHC	1.94	0.50
12:L:20:TRP:HZ3	27:L:102:LHG:H172	1.76	0.50
32:L:101:SQD:H251	32:L:101:SQD:H92	1.92	0.50
4:b:283:GLU:OE2	4:b:286:ARG:NH2	2.39	0.50
8:n:211:LEU:CD1	24:n:610:CLA:H3A	2.42	0.50
24:n:614:CLA:HBA1	24:n:614:CLA:HBD	1.94	0.50
24:a:407:CLA:O1A	24:a:407:CLA:H3A	2.12	0.50
34:c:517:DGD:HB22	30:c:518:LMG:H291	1.94	0.50
24:Aw:102:CLA:H191	20:R:120:LEU:HB3	1.94	0.50
8:A2:169:MET:HA	8:A2:172:VAL:HG22	1.92	0.50
24:A2:610:CLA:HBB1	24:A2:610:CLA:HMB3	1.94	0.50
14:A6:118:ALA:HB1	14:A6:229:GLY:HA3	1.94	0.50
4:BE:60:MET:CE	4:BE:63:ILE:HD12	2.40	0.50
5:D:266:ARG:HH12	20:A:220:THR:CG2	2.15	0.49
4:b:224:ARG:HH21	4:b:227:LYS:HZ3	1.58	0.49
14:s:221:LEU:HB3	24:s:609:CLA:CMA	2.41	0.49
8:y:231:VAL:HG11	24:y:314:CLA:HAC2	1.93	0.49
21:c:362:ARG:HD2	21:c:370:ARG:NH1	2.25	0.49
2:0:114:GLU:OE2	2:0:128:VAL:HA	2.12	0.49
24:0:602:CLA:CBB	25:0:616:LUT:H32	2.42	0.49
8:A2:90:GLU:N	8:A2:90:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BV:189:ARG:HH22	24:BV:608:CLA:H2A	1.77	0.49
22:BU:166:GLN:OE1	22:BU:166:GLN:N	2.35	0.49
22:BU:250:MET:HE2	24:BU:602:CLA:HMC1	1.94	0.49
22:BU:258:VAL:HG11	24:BU:612:CLA:CAC	2.40	0.49
23:BU:605:CHL:HMC	23:BU:606:CHL:C4C	2.42	0.49
2:6:126:GLU:OE1	2:6:135:GLN:NE2	2.44	0.49
5:D:137:VAL:CG2	5:D:139:LEU:HD23	2.40	0.49
6:e:27:ILE:HB	6:e:28:PRO:HD3	1.94	0.49
24:a:405:CLA:HBD	24:a:406:CLA:HAC2	1.94	0.49
1:9:101:ILE:HG22	23:9:609:CHL:HMD2	1.94	0.49
2:0:162:PHE:CE2	2:0:166:LEU:HD21	2.47	0.49
2:0:167:MET:SD	2:0:171:GLU:HG3	2.52	0.49
21:BF:367:GLU:HA	21:BF:370:ARG:HD2	1.93	0.49
1:5:238:LYS:HB2	1:5:242:GLU:OE1	2.12	0.49
3:8:106:GLY:HA3	3:8:232:SER:HB3	1.94	0.49
24:B:604:CLA:H172	27:B:621:LHG:H311	1.94	0.49
14:S:120:TRP:CE2	23:S:607:CHL:HED2	2.47	0.49
24:b:610:CLA:HMA2	24:b:611:CLA:C2C	2.43	0.49
24:g:611:CLA:H2	24:g:612:CLA:HED3	1.93	0.49
24:y:311:CLA:H52	25:y:316:LUT:H28	1.93	0.49
21:C:153:ASP:O	21:C:157:MET:HG2	2.12	0.49
24:r:610:CLA:NC	27:r:618:LHG:HC41	2.27	0.49
24:9:603:CLA:C2D	23:9:609:CHL:H52	2.41	0.49
9:Av:18:THR:O	9:Av:21:LYS:HG2	2.12	0.49
15:A7:8:PHE:CE1	29:BE:601:BCR:H361	2.47	0.49
24:BB:311:CLA:CHB	24:BB:311:CLA:H2	2.42	0.49
8:BQ:113:CYS:SG	25:BQ:616:LUT:H182	2.52	0.49
23:BQ:601:CHL:HED3	24:BQ:602:CLA:HBC2	1.93	0.49
8:Ba:90:GLU:O	8:Ba:94:ARG:HG2	2.13	0.49
23:Ba:307:CHL:OMC	25:Ba:317:LUT:H163	2.12	0.49
22:BU:219:GLY:O	22:BU:223:PHE:HB2	2.13	0.49
2:6:108:PHE:C	2:6:108:PHE:CD2	2.90	0.49
23:G:609:CHL:HHC	23:G:609:CHL:HBB1	1.94	0.49
4:b:359:MET:HE3	4:b:363:PHE:O	2.13	0.49
24:y:303:CLA:H61	25:y:317:LUT:H28	1.94	0.49
5:2:233:PHE:CE1	20:R:269:ARG:NE	2.80	0.49
8:A2:113:CYS:HG	8:A2:131:TRP:CG	2.30	0.49
5:BG:351:ASN:ND2	20:BD:336:ALA:O	2.45	0.49
9:BK:47:MET:HE1	29:BK:101:BCR:H312	1.93	0.49
14:BV:123:LEU:CG	24:BV:604:CLA:HAB	2.40	0.49
27:6:617:LHG:H271	27:6:617:LHG:HC91	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:458:PHE:HB3	24:B:604:CLA:HBC2	1.93	0.49
29:b:601:BCR:HC42	32:A:413:SQD:H152	1.94	0.49
8:n:103:SER:HB2	8:n:219:GLY:HA3	1.95	0.49
8:n:113:CYS:SG	25:n:616:LUT:H182	2.52	0.49
23:s:607:CHL:HBC2	23:s:607:CHL:HHD	1.93	0.49
8:y:146:TYR:OH	26:y:318:NEX:O23	2.27	0.49
24:y:304:CLA:CAD	23:y:310:CHL:H2	2.43	0.49
21:c:180:LEU:HD11	21:c:202:LEU:HD11	1.95	0.49
30:c:501:LMG:H221	24:c:504:CLA:HBB1	1.94	0.49
22:r:219:GLY:O	22:r:223:PHE:HB2	2.12	0.49
2:0:156:ILE:O	2:0:160:LEU:HG	2.13	0.49
2:0:197:LEU:CD1	25:0:615:LUT:H222	2.43	0.49
8:Au:202:ALA:HB2	24:Au:610:CLA:HAA2	1.94	0.49
8:A2:227:PHE:O	8:A2:231:VAL:HG22	2.12	0.49
19:BC:1:MET:SD	19:BC:1:MET:C	2.95	0.49
19:BC:57:LEU:O	19:BC:60:LEU:HG	2.12	0.49
23:BV:607:CHL:HHD	23:BV:607:CHL:HBC2	1.93	0.49
24:Ba:303:CLA:H61	25:Ba:317:LUT:H28	1.95	0.49
21:BF:180:LEU:HD11	21:BF:202:LEU:HD11	1.94	0.49
25:7:316:LUT:C8	25:7:316:LUT:H181	2.43	0.49
14:S:113:PHE:HD1	24:S:608:CLA:HED1	1.77	0.49
5:d:153:VAL:HG23	24:d:401:CLA:HED3	1.95	0.49
5:d:158:PHE:CE2	5:d:174:PHE:CE1	2.99	0.49
5:d:162:PRO:HB3	5:d:171:ALA:HB2	1.94	0.49
6:e:74:GLU:OE1	6:e:74:GLU:N	2.34	0.49
20:a:331:MET:HE2	20:a:331:MET:HA	1.93	0.49
1:9:155:ALA:HA	23:9:605:CHL:CHC	2.42	0.49
23:0:606:CHL:HBB1	25:0:616:LUT:H161	1.94	0.49
5:2:233:PHE:CD1	20:R:269:ARG:CZ	2.94	0.49
23:BB:310:CHL:C9	23:BB:310:CHL:C11	2.90	0.49
4:BE:201:HIS:HB2	24:BE:603:CLA:C1B	2.42	0.49
24:BQ:614:CLA:HBD	24:BQ:614:CLA:HBA1	1.94	0.49
28:BQ:619:XAT:H203	24:Ba:314:CLA:H52	1.94	0.49
14:BV:160:LEU:H	14:BV:160:LEU:HD12	1.78	0.49
2:6:162:PHE:CE1	2:6:166:LEU:HD11	2.47	0.49
1:7:169:MET:HA	1:7:172:VAL:HG22	1.94	0.49
5:D:60:TYR:HB3	6:E:66:ILE:HD11	1.94	0.49
23:g:607:CHL:H191	23:n:601:CHL:H41	1.93	0.49
14:s:189:ARG:HH22	24:s:608:CLA:H2A	1.77	0.49
19:z:44:THR:O	19:z:48:ILE:HG12	2.13	0.49
20:a:183:MET:HE1	24:a:406:CLA:HHD	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:76:VAL:CG1	21:c:79:LYS:HZ3	2.23	0.49
2:0:126:GLU:OE1	2:0:135:GLN:NE2	2.45	0.49
2:0:253:ASN:HB2	24:0:614:CLA:HED1	1.94	0.49
24:AA:304:CLA:C2D	23:AA:310:CHL:H52	2.43	0.49
4:v:106:LEU:HD21	29:v:619:BCR:C16	2.43	0.49
9:Av:62:ASN:HA	34:Av:102:DGD:HG2	1.95	0.49
14:A6:113:PHE:HD1	24:A6:608:CLA:HED1	1.78	0.49
14:BV:154:LEU:HG	14:BV:171:LEU:HG	1.94	0.49
20:R:308:ASP:OD1	20:R:312:ARG:N	2.40	0.49
20:BD:134:SER:HA	20:BD:139:MET:HE2	1.94	0.49
24:BD:405:CLA:C3	38:BD:408:PHO:HBB1	2.43	0.49
1:5:161:ILE:HD11	23:5:606:CHL:C2D	2.42	0.49
24:7:304:CLA:C2D	23:7:310:CHL:H52	2.43	0.49
14:S:122:MET:HE1	24:S:609:CLA:HHC	1.94	0.49
34:C:517:DGD:HB31	30:C:519:LMG:H321	1.95	0.49
22:r:125:GLN:HG2	22:r:125:GLN:O	2.12	0.49
22:r:216:LEU:C	22:r:216:LEU:HD12	2.37	0.49
22:r:283:ILE:O	22:r:286:THR:OG1	2.26	0.49
2:0:173:PHE:CD2	2:0:178:LEU:HD11	2.48	0.49
1:AA:121:ARG:HH12	1:AA:242:GLU:N	2.10	0.49
5:2:232:THR:C	20:R:269:ARG:NH1	2.71	0.49
5:2:266:ARG:NH2	5:2:270:PHE:N	2.61	0.49
8:A2:80:TRP:CD1	8:A2:82:THR:HG23	2.47	0.49
8:A2:113:CYS:SG	8:A2:131:TRP:CG	3.06	0.49
17:A0:100:LEU:O	17:A0:104:ILE:HG12	2.13	0.49
24:BE:610:CLA:HMA2	24:BE:611:CLA:C2C	2.43	0.49
19:Bb:44:THR:O	19:Bb:48:ILE:HG12	2.13	0.49
3:8:144:SER:O	3:8:148:THR:HG22	2.13	0.49
3:8:157:GLU:HG2	3:8:160:ARG:NH1	2.28	0.49
8:G:149:ASN:HB3	8:G:152:LEU:HG	1.95	0.49
14:S:118:ALA:HB1	14:S:229:GLY:HA3	1.93	0.49
14:S:160:LEU:HD11	24:S:604:CLA:HAA1	1.95	0.49
17:W:101:LEU:HD23	17:W:104:ILE:HD11	1.95	0.49
27:d:404:LHG:H321	15:t:21:ILE:HD11	1.94	0.49
11:k:40:MET:HA	11:k:43:ILE:HD13	1.93	0.49
8:n:97:GLU:OE2	23:n:609:CHL:HED1	2.12	0.49
1:9:106:ALA:HA	1:9:226:MET:HE1	1.93	0.49
24:9:602:CLA:H52	25:9:616:LUT:H28	1.94	0.49
2:0:161:GLY:O	2:0:165:ILE:HG12	2.13	0.49
1:AA:232:GLN:O	1:AA:236:THR:HG22	2.13	0.49
4:v:151:PHE:C	4:v:151:PHE:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:613:CLA:H91	24:v:613:CLA:H111	1.62	0.49
12:Az:27:VAL:HG21	27:Az:102:LHG:H192	1.94	0.49
13:BP:2:GLU:O	13:BP:3:VAL:HG22	2.12	0.49
8:BQ:169:MET:SD	23:BQ:609:CHL:C1C	3.01	0.49
21:BF:157:MET:N	21:BF:157:MET:SD	2.86	0.49
22:BU:148:MET:SD	25:BU:615:LUT:C35	3.01	0.49
1:5:162:TRP:HE1	28:5:619:XAT:C14	2.26	0.49
23:5:601:CHL:HAC2	27:5:618:LHG:HC32	1.94	0.49
28:5:619:XAT:H382	23:6:601:CHL:C1C	2.43	0.49
2:6:242:LEU:HD21	25:6:615:LUT:C2	2.43	0.49
23:G:601:CHL:H62	23:G:601:CHL:H41	1.66	0.49
24:N:610:CLA:HBB1	24:N:610:CLA:HMB3	1.95	0.49
4:b:63:ILE:N	4:b:64:PRO:HD2	2.28	0.49
4:b:226:TYR:HD2	4:b:231:MET:HB2	1.74	0.49
25:AA:316:LUT:H181	25:AA:316:LUT:C8	2.42	0.49
7:4:28:LEU:O	7:4:32:SER:OG	2.28	0.49
4:BE:92:SER:OG	4:BE:94:GLU:OE1	2.27	0.49
24:BE:602:CLA:HAC1	29:BK:101:BCR:H383	1.94	0.49
5:BG:265:LYS:CE	20:BD:245:THR:HG22	2.43	0.49
14:BV:203:GLY:HA2	14:BV:207:ASP:OD2	2.13	0.49
14:BV:221:LEU:HD13	14:BV:224:LYS:HG3	1.94	0.49
24:1:512:CLA:H161	24:1:513:CLA:H13	1.93	0.49
20:BD:37:MET:SD	20:BD:41:LEU:HD12	2.53	0.49
20:BD:61:ASP:OD2	20:BD:61:ASP:N	2.38	0.49
20:BD:333:GLU:HB3	20:BD:336:ALA:HB2	1.95	0.49
2:6:234:THR:HG21	2:6:241:ASN:ND2	2.28	0.48
1:7:121:ARG:HH12	1:7:242:GLU:N	2.10	0.48
24:8:301:CLA:CBB	28:8:312:XAT:H32	2.43	0.48
4:B:384:ARG:HB2	5:D:353:LEU:HD22	1.94	0.48
18:X:78:GLY:C	18:X:80:SER:H	2.21	0.48
4:b:41:GLU:CD	4:b:62:VAL:HG22	2.38	0.48
4:b:231:MET:HE1	24:b:611:CLA:HMC1	1.94	0.48
9:h:29:GLU:HG3	9:h:32:LYS:HB3	1.95	0.48
14:s:167:ILE:HG22	14:s:169:ILE:HG22	1.95	0.48
8:y:226:MET:HE3	8:y:226:MET:O	2.13	0.48
20:a:183:MET:HE2	24:a:406:CLA:HAC1	1.95	0.48
22:r:213:GLU:OE2	22:r:217:TYR:HB2	2.12	0.48
1:9:238:LYS:HB2	1:9:242:GLU:OE1	2.13	0.48
28:9:619:XAT:H382	23:0:601:CHL:C1C	2.43	0.48
24:AB:301:CLA:H3A	24:AB:301:CLA:HBA2	1.35	0.48
4:v:57:ARG:HD2	4:v:330:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:223:GLN:NE2	4:v:224:ARG:HG3	2.28	0.48
8:Au:107:MET:HE1	24:Au:610:CLA:HHC	1.93	0.48
8:Au:117:GLU:OE2	8:Au:242:GLU:HG2	2.12	0.48
24:A6:602:CLA:H61	25:A6:615:LUT:H373	1.95	0.48
4:BE:250:PHE:CE2	34:BK:102:DGD:HBT1	2.48	0.48
8:BJ:224:PHE:CE2	24:BJ:613:CLA:HAB	2.47	0.48
24:BD:407:CLA:H3A	24:BD:407:CLA:O1A	2.12	0.48
2:6:102:TRP:CD1	23:6:609:CHL:HMD3	2.48	0.48
4:B:169:SER:OG	4:B:266:GLU:OE1	2.30	0.48
14:s:233:MET:HE3	24:s:602:CLA:C1C	2.43	0.48
24:a:405:CLA:C3	38:a:408:PHO:HBB1	2.43	0.48
24:c:502:CLA:HHC	24:c:502:CLA:HBB1	1.95	0.48
3:AB:144:SER:O	3:AB:148:THR:HG22	2.13	0.48
8:Au:160:ALA:O	8:Au:164:THR:HG23	2.12	0.48
9:Av:47:MET:HE1	29:Av:101:BCR:HC8	1.95	0.48
29:BE:601:BCR:HC42	32:R:411:SQD:H152	1.95	0.48
21:BF:39:ASN:HB2	24:BF:509:CLA:HBA1	1.95	0.48
22:BU:138:GLU:O	22:BU:142:ILE:HG22	2.13	0.48
4:B:256:MET:HE1	4:B:263:THR:OG1	2.13	0.48
5:D:233:PHE:CD1	20:A:269:ARG:HD3	2.48	0.48
5:d:187:GLN:HB2	24:d:401:CLA:HBC1	1.95	0.48
24:n:613:CLA:H91	27:n:618:LHG:H321	1.95	0.48
14:s:69:ILE:HD11	14:s:78:ARG:NH1	2.28	0.48
23:y:310:CHL:H192	23:y:310:CHL:H161	1.72	0.48
22:r:141:LEU:HD21	22:r:145:ARG:CZ	2.43	0.48
24:AB:302:CLA:HBC3	28:AB:312:XAT:C12	2.43	0.48
4:v:458:PHE:HB3	24:v:604:CLA:HBC2	1.96	0.48
5:2:60:TYR:HB3	6:3:66:ILE:HD11	1.94	0.48
5:2:200:MET:HE1	5:2:282:MET:SD	2.54	0.48
12:Az:20:TRP:HZ3	27:Az:102:LHG:H172	1.78	0.48
8:A2:76:GLY:HA3	8:A2:216:LEU:HD23	1.94	0.48
26:BB:320:NEX:H382	24:BU:604:CLA:H12	1.94	0.48
4:BE:25:MET:CE	29:BE:618:BCR:H393	2.42	0.48
6:BH:27:ILE:HB	6:BH:28:PRO:HD3	1.95	0.48
24:BQ:613:CLA:H91	27:BQ:618:LHG:H321	1.95	0.48
14:BV:115:LEU:HD21	14:BV:119:ARG:NH2	2.28	0.48
23:5:606:CHL:HBC2	23:5:607:CHL:HHD	1.95	0.48
4:b:247:PHE:HE1	24:b:603:CLA:H122	1.77	0.48
8:g:176:ARG:NH2	23:g:609:CHL:O1D	2.35	0.48
8:n:169:MET:SD	23:n:609:CHL:C2C	3.02	0.48
14:s:154:LEU:HG	14:s:171:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:25:GLU:N	20:a:25:GLU:OE2	2.46	0.48
24:r:609:CLA:H2	25:r:615:LUT:H26	1.94	0.48
24:0:602:CLA:H142	25:0:616:LUT:H393	1.95	0.48
24:AA:312:CLA:C4D	24:AA:313:CLA:HMD3	2.43	0.48
4:v:201:HIS:HB2	24:v:602:CLA:CHB	2.43	0.48
24:Aw:102:CLA:H61	24:Aw:102:CLA:H92	1.60	0.48
13:A1:6:LEU:H	13:A1:6:LEU:HD12	1.79	0.48
8:BB:100:VAL:O	8:BB:103:SER:OG	2.28	0.48
24:BB:305:CLA:HBA2	24:BB:305:CLA:H3A	1.40	0.48
23:BJ:601:CHL:H202	23:BJ:601:CHL:H161	1.69	0.48
18:BZ:97:LEU:O	18:BZ:101:ILE:HG12	2.14	0.48
29:Bb:101:BCR:H323	21:BF:116:VAL:HG23	1.95	0.48
22:BU:153:GLY:O	22:BU:157:VAL:HG12	2.12	0.48
1:5:196:PHE:O	25:5:615:LUT:H24	2.13	0.48
24:B:614:CLA:HMB1	24:B:614:CLA:HBB1	1.96	0.48
24:B:616:CLA:OBD	9:H:17:THR:HG21	2.13	0.48
24:Y:312:CLA:CGA	27:C:520:LHG:HC5	2.44	0.48
6:e:37:PHE:CD1	6:e:37:PHE:C	2.92	0.48
22:r:189:SER:OG	22:r:190:THR:N	2.46	0.48
23:r:605:CHL:H193	23:r:607:CHL:HBB2	1.95	0.48
8:A2:220:ARG:HD3	24:A2:602:CLA:CHD	2.42	0.48
23:A2:607:CHL:H121	23:BB:302:CHL:H18	1.95	0.48
25:A2:616:LUT:H181	25:A2:616:LUT:H8	1.96	0.48
4:BE:41:GLU:CB	4:BE:60:MET:HE1	2.39	0.48
8:Ba:119:LEU:HD12	8:Ba:124:VAL:HG21	1.95	0.48
8:Ba:186:ALA:HB2	23:Ba:309:CHL:HBC1	1.96	0.48
21:BF:134:LEU:HG	21:BF:135:LEU:HD23	1.94	0.48
34:BF:518:DGD:HB22	30:BF:519:LMG:H291	1.95	0.48
24:8:308:CLA:HMC1	25:8:311:LUT:H402	1.95	0.48
8:G:202:ALA:HB2	24:G:610:CLA:HAA2	1.95	0.48
9:H:65:VAL:HG23	9:H:67:LEU:HB3	1.94	0.48
8:N:97:GLU:HG3	8:N:190:LEU:HD21	1.95	0.48
17:W:92:LEU:HD22	17:W:97:SER:HA	1.94	0.48
8:g:226:MET:HE1	25:g:616:LUT:C10	2.40	0.48
10:i:2:LEU:O	10:i:6:LEU:HD22	2.14	0.48
13:m:1:MET:SD	13:m:2:GLU:N	2.87	0.48
14:s:209:LEU:HD12	25:s:614:LUT:H222	1.95	0.48
8:y:186:ALA:HB2	23:y:309:CHL:HBC1	1.96	0.48
1:9:100:VAL:HG11	1:9:190:LEU:HG	1.94	0.48
2:0:48:TYR:HE2	2:0:207:ALA:HB1	1.79	0.48
24:v:602:CLA:H93	24:v:602:CLA:H61	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A2:607:CHL:H3A	23:A2:607:CHL:HBA1	1.43	0.48
14:A6:73:ASP:OD2	14:A6:74:GLY:N	2.47	0.48
34:BK:102:DGD:HB62	34:BK:102:DGD:HB91	1.50	0.48
12:BO:15:ARG:HH12	32:BO:101:SQD:H462	1.78	0.48
19:Bb:22:SER:O	19:Bb:26:VAL:HG12	2.14	0.48
20:BD:104:GLU:OE2	20:BD:108:ASN:ND2	2.46	0.48
21:BF:346:THR:OG1	21:BF:348:GLU:OE1	2.26	0.48
24:BU:610:CLA:NC	27:BU:617:LHG:HC41	2.27	0.48
23:G:601:CHL:HHC	23:G:601:CHL:HBB1	1.96	0.48
24:G:613:CLA:H102	28:Y:301:XAT:H15	1.96	0.48
8:N:176:ARG:NH2	23:N:609:CHL:O1D	2.39	0.48
23:N:601:CHL:HBA1	23:N:601:CHL:H3A	1.42	0.48
24:Y:312:CLA:H3A	24:Y:312:CLA:HBA2	1.48	0.48
4:b:367:PRO:HB2	5:d:346:VAL:CG1	2.44	0.48
24:b:602:CLA:HAC1	29:h:101:BCR:H383	1.94	0.48
8:n:121:ARG:NH1	8:n:121:ARG:O	2.47	0.48
16:u:79:ARG:HG2	16:u:99:LYS:O	2.13	0.48
19:z:22:SER:O	19:z:26:VAL:HG12	2.14	0.48
24:c:506:CLA:H92	24:c:506:CLA:H61	1.70	0.48
15:A7:6:TYR:HA	15:A7:9:LEU:HD12	1.95	0.48
18:BA:78:GLY:C	18:BA:80:SER:H	2.20	0.48
24:BB:311:CLA:H102	24:BB:311:CLA:H13	1.69	0.48
24:BG:401:CLA:H41	24:BG:401:CLA:H62	1.54	0.48
12:BO:12:GLU:HA	13:BP:29:THR:CG2	2.44	0.48
8:Ba:231:VAL:HG11	24:Ba:314:CLA:HAC2	1.94	0.48
24:Ba:304:CLA:CAD	23:Ba:310:CHL:H2	2.44	0.48
4:B:348:ASN:OD1	4:B:352:ARG:N	2.45	0.48
23:Y:310:CHL:C9	23:Y:310:CHL:C11	2.91	0.48
8:n:106:ALA:CB	8:n:223:MET:SD	3.01	0.48
20:a:183:MET:HB3	24:a:405:CLA:HBC2	1.96	0.48
22:r:158:GLU:OE2	22:r:268:LEU:HG	2.13	0.48
2:0:169:LEU:O	2:0:173:PHE:CD1	2.66	0.48
8:A2:151:SER:HB3	14:A6:139:ALA:HB2	1.96	0.48
8:BB:226:MET:CG	25:BB:317:LUT:H12	2.41	0.48
4:BE:63:ILE:N	4:BE:64:PRO:HD2	2.29	0.48
4:BE:324:LEU:HA	5:BG:294:LEU:HD12	1.96	0.48
4:BE:468:TRP:NE1	4:BE:472:ARG:HH21	2.11	0.48
8:BJ:100:VAL:O	8:BJ:103:SER:OG	2.28	0.48
8:BQ:95:ASN:HD21	24:BQ:602:CLA:H12	1.78	0.48
15:BW:10:LEU:O	15:BW:14:LEU:HD23	2.13	0.48
24:BF:509:CLA:HBA2	24:BF:509:CLA:H3A	1.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:161:ILE:O	1:5:165:GLN:HG2	2.13	0.48
2:6:91:LYS:HE3	1:7:82:THR:O	2.12	0.48
24:6:602:CLA:H142	25:6:616:LUT:H393	1.95	0.48
23:7:302:CHL:HBA1	23:7:302:CHL:H3A	1.61	0.48
23:7:310:CHL:HHC	23:7:310:CHL:HBB1	1.96	0.48
3:8:221:LEU:O	3:8:225:LYS:HG3	2.14	0.48
3:8:228:GLU:O	3:8:232:SER:OG	2.32	0.48
8:Y:186:ALA:HB2	23:Y:309:CHL:HBC1	1.95	0.48
24:b:603:CLA:H102	24:b:610:CLA:H193	1.95	0.48
24:y:313:CLA:HMC3	25:y:316:LUT:H191	1.95	0.48
20:a:143:ILE:H	20:a:143:ILE:HD12	1.78	0.48
1:9:227:PHE:O	1:9:231:VAL:HG12	2.14	0.48
3:AB:239:MET:HE3	3:AB:243:TYR:HB2	1.96	0.48
10:Aw:7:PHE:O	10:Aw:11:VAL:HG22	2.14	0.48
32:Az:101:SQD:H142	32:BO:101:SQD:H383	1.96	0.48
14:A6:122:MET:HE1	24:A6:609:CLA:HHC	1.94	0.48
4:BE:223:GLN:HB2	4:BE:224:ARG:NH1	2.29	0.48
14:BV:186:GLU:O	14:BV:190:ILE:HG22	2.14	0.48
2:6:238:PRO:O	2:6:242:LEU:HD23	2.14	0.48
4:B:201:HIS:HB2	24:B:602:CLA:CHB	2.44	0.48
4:B:223:GLN:NE2	4:B:224:ARG:HG3	2.29	0.48
8:G:160:ALA:O	8:G:164:THR:HG23	2.13	0.48
4:b:188:GLU:OE1	4:b:188:GLU:N	2.36	0.48
24:b:605:CLA:H193	24:b:617:CLA:H201	1.96	0.48
24:b:615:CLA:HBB1	24:b:615:CLA:HMB1	1.95	0.48
5:d:25:ARG:NH2	5:d:26:ASP:HB3	2.28	0.48
23:g:605:CHL:H3A	23:g:605:CHL:HBA2	1.63	0.48
24:g:613:CLA:H91	27:g:618:LHG:H321	1.96	0.48
23:9:601:CHL:HAC2	27:9:618:LHG:HC32	1.94	0.48
24:0:602:CLA:H3A	24:0:602:CLA:O2A	2.14	0.48
1:AA:239:GLY:O	1:AA:243:ASN:ND2	2.39	0.48
5:2:232:THR:N	20:R:269:ARG:HH12	2.11	0.48
23:Au:606:CHL:HAA1	23:Au:606:CHL:CGD	2.44	0.48
4:BE:384:ARG:HA	4:BE:385:ARG:NH1	2.29	0.48
1:5:107:MET:HE2	24:5:610:CLA:HHC	1.94	0.47
1:5:178:ALA:HA	2:6:62:GLN:HE22	1.79	0.47
24:5:602:CLA:H52	25:5:616:LUT:H28	1.95	0.47
1:7:168:LEU:CD1	26:7:319:NEX:H34	2.43	0.47
1:7:202:ALA:HB2	24:7:311:CLA:HAA2	1.96	0.47
25:G:616:LUT:C8	25:G:616:LUT:H181	2.44	0.47
23:N:608:CHL:H152	26:N:617:NEX:H402	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:607:CLA:H72	29:b:620:BCR:H321	1.96	0.47
5:d:233:PHE:HB3	32:d:406:SQD:H5	1.96	0.47
8:g:227:PHE:HE1	24:g:602:CLA:H18	1.78	0.47
8:n:111:LEU:HA	8:n:114:VAL:HG12	1.95	0.47
23:n:601:CHL:H3A	23:n:601:CHL:HBA1	1.53	0.47
14:s:123:LEU:CG	24:s:604:CLA:HAB	2.42	0.47
14:s:189:ARG:NH2	24:s:608:CLA:O1D	2.47	0.47
24:C:511:CLA:O2D	24:C:511:CLA:H2A	2.14	0.47
21:c:157:MET:SD	21:c:157:MET:N	2.87	0.47
22:r:134:GLN:OE1	22:r:134:GLN:N	2.43	0.47
22:r:141:LEU:C	22:r:141:LEU:HD23	2.38	0.47
22:r:231:ASP:HB3	22:r:234:LYS:NZ	2.29	0.47
1:9:113:CYS:HG	1:9:131:TRP:CG	2.32	0.47
4:v:258:TYR:CD2	34:Av:102:DGD:HG31	2.49	0.47
5:2:159:LEU:O	5:2:163:LEU:HG	2.14	0.47
23:A2:608:CHL:H152	26:A2:617:NEX:H402	1.95	0.47
5:BG:202:VAL:HG22	24:BG:401:CLA:C2B	2.44	0.47
9:BK:62:ASN:ND2	34:BK:102:DGD:O1G	2.47	0.47
2:6:253:ASN:HB2	24:6:614:CLA:HED1	1.95	0.47
5:D:56:VAL:HG21	5:D:111:LEU:HD12	1.96	0.47
23:G:606:CHL:HAA1	23:G:606:CHL:CGD	2.44	0.47
24:I:102:CLA:H61	24:I:102:CLA:H92	1.60	0.47
24:b:603:CLA:H101	9:h:58:LEU:HD12	1.96	0.47
24:b:606:CLA:HBB1	24:b:607:CLA:H51	1.96	0.47
5:d:111:LEU:HD12	5:d:111:LEU:H	1.79	0.47
24:c:505:CLA:H11	34:c:517:DGD:HB42	1.97	0.47
3:AB:204:GLY:HA3	3:AB:208:LYS:HE3	1.96	0.47
29:v:622:BCR:H313	15:BW:17:ILE:HG22	1.96	0.47
8:Au:182:PRO:HG2	26:Au:617:NEX:H192	1.96	0.47
24:A6:602:CLA:H3A	24:A6:602:CLA:HBA2	1.35	0.47
5:BG:75:LEU:H	5:BG:75:LEU:HD12	1.79	0.47
24:Ba:305:CLA:HBA1	23:Ba:307:CHL:CHD	2.44	0.47
20:R:184:ILE:CG2	20:R:328:MET:HE3	2.35	0.47
21:1:42:LEU:HD21	24:1:511:CLA:HED1	1.96	0.47
1:5:76:GLY:HA3	1:5:216:LEU:HD13	1.96	0.47
4:B:150:CYS:SG	4:B:202:HIS:O	2.72	0.47
23:G:608:CHL:H143	23:G:608:CHL:H162	1.70	0.47
24:S:608:CLA:H3A	24:S:608:CLA:HBA2	1.48	0.47
24:b:613:CLA:H102	24:b:613:CLA:H61	1.59	0.47
5:d:284:ALA:O	5:d:288:VAL:HG23	2.14	0.47
23:g:601:CHL:HBA1	23:g:601:CHL:H3A	1.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:l:101:SQD:H342	32:l:101:SQD:H312	1.52	0.47
23:n:609:CHL:C9	23:n:609:CHL:H112	2.43	0.47
8:y:88:ASP:OD1	8:y:89:PRO:CD	2.62	0.47
21:C:198:LYS:HD3	21:C:198:LYS:HA	1.71	0.47
23:r:607:CHL:HBB1	23:r:607:CHL:HHC	1.96	0.47
1:AA:107:MET:HE1	25:AA:316:LUT:C33	2.45	0.47
3:AB:71:GLU:H	3:AB:71:GLU:CD	2.23	0.47
24:AB:310:CLA:HBA2	24:AB:310:CLA:CBD	2.42	0.47
29:v:622:BCR:HC7	15:BW:18:PHE:HB2	1.96	0.47
25:Au:616:LUT:C8	25:Au:616:LUT:H181	2.44	0.47
4:BE:151:PHE:CE2	4:BE:203:ILE:HG23	2.49	0.47
21:1:180:LEU:HD11	21:1:202:LEU:HD21	1.94	0.47
21:BF:223:TRP:CG	21:BF:224:ILE:H	2.32	0.47
24:BF:514:CLA:H92	27:BF:521:LHG:H122	1.96	0.47
1:5:158:ILE:HG12	2:6:255:TRP:CZ3	2.49	0.47
23:6:601:CHL:C9	23:6:601:CHL:H62	2.44	0.47
4:B:258:TYR:CD2	34:H:102:DGD:HG31	2.49	0.47
34:H:102:DGD:HB81	34:H:102:DGD:HB51	1.64	0.47
11:K:40:MET:HA	11:K:43:ILE:HG12	1.95	0.47
4:b:216:HIS:CE1	24:b:610:CLA:C1A	2.98	0.47
9:h:62:ASN:ND2	34:h:102:DGD:O1G	2.47	0.47
23:n:601:CHL:H41	23:n:601:CHL:H62	1.65	0.47
21:c:71:GLU:CG	21:c:89:LEU:HD13	2.36	0.47
1:9:107:MET:CE	24:9:610:CLA:HHC	2.44	0.47
1:9:107:MET:HE3	25:9:615:LUT:H34	1.97	0.47
1:AA:61:PRO:HD2	23:AA:302:CHL:CBB	2.44	0.47
4:v:54:PRO:HD2	4:v:57:ARG:HG3	1.95	0.47
4:v:216:HIS:HE1	24:v:609:CLA:C1A	2.27	0.47
14:A6:217:GLN:N	14:A6:217:GLN:OE1	2.47	0.47
4:BE:155:ALA:C	4:BE:156:PHE:HD1	2.23	0.47
24:BE:615:CLA:HMB1	24:BE:615:CLA:HBB1	1.95	0.47
5:BG:19:MET:HE1	18:BZ:102:GLY:C	2.39	0.47
23:BJ:601:CHL:HED3	24:BJ:602:CLA:HBC1	1.96	0.47
10:BL:2:LEU:O	10:BL:6:LEU:HD22	2.14	0.47
22:BU:207:ASN:ND2	24:BU:614:CLA:HHD	2.30	0.47
2:6:161:GLY:O	2:6:165:ILE:HG12	2.14	0.47
2:6:224:MET:CE	2:6:227:PHE:HD2	2.27	0.47
3:8:239:MET:HE3	3:8:243:TYR:HB2	1.96	0.47
5:D:159:LEU:O	5:D:163:LEU:HG	2.14	0.47
15:T:15:GLY:HA2	29:b:601:BCR:H12C	1.96	0.47
23:Y:306:CHL:HAA1	23:Y:306:CHL:HBD	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:603:CLA:H93	24:b:603:CLA:H61	1.68	0.47
5:d:153:VAL:HG23	24:d:401:CLA:CED	2.45	0.47
23:g:606:CHL:HBB2	23:g:607:CHL:CBB	2.45	0.47
9:h:32:LYS:HD2	9:h:32:LYS:HA	1.64	0.47
22:r:138:GLU:O	22:r:142:ILE:HG22	2.14	0.47
28:9:619:XAT:O3	2:0:261:PHE:HB2	2.14	0.47
2:0:68:THR:OG1	2:0:70:GLU:OE1	2.27	0.47
2:0:224:MET:CE	2:0:227:PHE:HD2	2.28	0.47
13:A1:1:MET:HE3	13:A1:2:GLU:H	1.78	0.47
8:A2:107:MET:HE3	25:A2:615:LUT:C34	2.44	0.47
24:A6:602:CLA:H102	25:A6:615:LUT:H371	1.95	0.47
16:A8:82:GLU:O	16:A8:86:LYS:HG2	2.14	0.47
17:A0:110:GLY:HA3	27:A0:202:LHG:H181	1.96	0.47
23:BJ:607:CHL:CBB	25:BJ:616:LUT:H193	2.45	0.47
14:BV:159:THR:OG1	14:BV:166:ASN:OD1	2.33	0.47
21:1:153:ASP:O	21:1:157:MET:HG2	2.14	0.47
20:BD:143:ILE:H	20:BD:143:ILE:HD12	1.79	0.47
21:BF:57:ALA:O	21:BF:61:VAL:HG23	2.15	0.47
23:BU:605:CHL:H3A	23:BU:605:CHL:HBA2	1.65	0.47
1:7:223:MET:SD	1:7:223:MET:C	2.97	0.47
29:B:623:BCR:HC7	15:t:18:PHE:HB2	1.97	0.47
8:G:107:MET:HE3	25:G:615:LUT:C34	2.45	0.47
24:G:602:CLA:H3A	24:G:602:CLA:HBA2	1.40	0.47
11:K:54:TRP:HH2	24:C:511:CLA:C3D	2.27	0.47
14:S:241:ILE:HG21	24:S:612:CLA:HAC2	1.96	0.47
8:Y:175:TYR:CE1	8:Y:182:PRO:HD3	2.50	0.47
5:d:55:PHE:HB3	6:e:47:PHE:HD1	1.78	0.47
8:g:65:GLU:N	8:g:65:GLU:OE1	2.47	0.47
24:n:610:CLA:H3A	24:n:610:CLA:HBA2	1.72	0.47
14:s:186:GLU:O	14:s:190:ILE:HG22	2.14	0.47
21:c:346:THR:OG1	21:c:348:GLU:OE1	2.25	0.47
22:r:157:VAL:O	22:r:161:THR:HG22	2.14	0.47
23:9:609:CHL:C3B	23:0:601:CHL:H2	2.44	0.47
1:AA:59:LEU:HB2	1:AA:63:SER:HA	1.95	0.47
1:AA:241:LEU:O	1:AA:244:LEU:HG	2.14	0.47
23:AB:307:CHL:HBB1	23:AB:307:CHL:HHC	1.97	0.47
23:A2:606:CHL:OMC	25:A2:616:LUT:H163	2.15	0.47
23:BB:306:CHL:HAA1	23:BB:306:CHL:HBD	1.95	0.47
23:BB:310:CHL:C9	23:BB:310:CHL:C6	2.93	0.47
2:6:150:LEU:O	2:6:152:HIS:N	2.48	0.47
4:B:112:ILE:HG12	29:B:617:BCR:H271	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:8:GLU:HG2	32:L:101:SQD:H62	1.97	0.47
8:N:227:PHE:O	8:N:231:VAL:HG22	2.14	0.47
19:Z:3:ILE:O	19:Z:7:LEU:HG	2.14	0.47
4:b:237:VAL:HG11	24:b:611:CLA:HBC2	1.96	0.47
8:g:103:SER:HA	8:g:223:MET:HE2	1.97	0.47
9:h:56:ILE:O	9:h:60:ILE:HG12	2.15	0.47
11:k:42:VAL:HG12	11:k:46:PHE:CE1	2.49	0.47
13:m:2:GLU:O	13:m:3:VAL:HG22	2.15	0.47
23:y:307:CHL:HAA1	23:y:307:CHL:CGD	2.45	0.47
19:z:11:ALA:O	19:z:15:THR:HG22	2.14	0.47
20:A:172:MET:HE3	20:A:173:PRO:O	2.15	0.47
21:C:451:ALA:HA	21:C:456:GLU:CD	2.40	0.47
21:c:57:ALA:O	21:c:61:VAL:HG23	2.15	0.47
21:c:81:MET:CG	21:c:86:LEU:HD12	2.43	0.47
24:c:507:CLA:H12	29:c:515:BCR:H321	1.97	0.47
22:r:258:VAL:HG11	24:r:612:CLA:CAC	2.39	0.47
25:r:615:LUT:C8	25:r:615:LUT:H181	2.44	0.47
23:0:601:CHL:C9	23:0:601:CHL:H62	2.44	0.47
23:0:606:CHL:HBA2	23:0:606:CHL:H3A	1.55	0.47
1:AA:211:LEU:HB3	24:AA:311:CLA:HMA2	1.97	0.47
4:v:256:MET:HE2	4:v:256:MET:HA	1.95	0.47
24:v:604:CLA:H203	27:v:621:LHG:H341	1.97	0.47
5:2:56:VAL:HG21	5:2:111:LEU:HD12	1.97	0.47
23:A2:608:CHL:C9	23:A2:608:CHL:C11	2.93	0.47
25:BB:316:LUT:C8	25:BB:316:LUT:H181	2.44	0.47
4:BE:283:GLU:OE2	4:BE:286:ARG:NH2	2.40	0.47
24:BE:607:CLA:H72	29:BE:620:BCR:H321	1.95	0.47
9:BK:66:LEU:HD22	18:BZ:81:PRO:HG3	1.97	0.47
23:BQ:606:CHL:CBB	25:BQ:616:LUT:H161	2.44	0.47
24:BQ:610:CLA:H12	24:BQ:610:CLA:HBA2	1.46	0.47
24:BQ:613:CLA:HED2	24:BQ:613:CLA:HBD	1.74	0.47
18:BZ:94:GLY:O	18:BZ:97:LEU:HG	2.13	0.47
38:BD:408:PHO:H61	38:BD:408:PHO:H2	1.62	0.47
24:BF:509:CLA:H2	24:BF:511:CLA:H12	1.97	0.47
22:BU:273:THR:O	22:BU:276:SER:OG	2.26	0.47
1:5:152:LEU:O	1:5:154:HIS:N	2.48	0.47
24:6:602:CLA:H52	25:6:616:LUT:H28	1.96	0.47
23:6:606:CHL:HBB1	25:6:616:LUT:H161	1.97	0.47
3:8:127:TRP:HE1	3:8:252:PRO:CD	2.28	0.47
24:8:308:CLA:CGA	24:8:308:CLA:C3A	2.89	0.47
4:B:216:HIS:HE1	24:B:609:CLA:C1A	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:182:LEU:HD12	14:S:182:LEU:HA	1.72	0.47
14:S:186:GLU:O	14:S:190:ILE:HG22	2.15	0.47
24:S:609:CLA:H3A	24:S:609:CLA:CGA	2.45	0.47
4:b:169:SER:OG	4:b:266:GLU:OE1	2.27	0.47
24:b:605:CLA:H141	24:b:605:CLA:H161	1.70	0.47
12:l:15:ARG:HH12	32:l:101:SQD:H462	1.79	0.47
20:A:20:TRP:HE1	32:A:413:SQD:HO3	1.57	0.47
2:0:162:PHE:CE1	2:0:166:LEU:HD11	2.50	0.47
3:AB:228:GLU:CD	24:AB:308:CLA:HMA1	2.39	0.47
4:v:112:ILE:HG12	29:v:617:BCR:H271	1.96	0.47
24:v:609:CLA:H92	24:v:609:CLA:H61	1.75	0.47
27:Az:102:LHG:H142	27:Az:102:LHG:H112	1.64	0.47
24:BB:312:CLA:CGA	27:1:520:LHG:HC5	2.45	0.47
5:BG:78:ALA:HB2	5:BG:175:GLY:HA3	1.96	0.47
5:BG:219:VAL:HG11	20:BD:272:HIS:CG	2.49	0.47
17:BY:117:PHE:HA	17:BY:120:THR:HG22	1.97	0.47
32:R:411:SQD:H321	32:R:411:SQD:H291	1.48	0.47
20:BD:204:GLY:HA2	20:BD:278:TRP:NE1	2.30	0.47
23:BU:607:CHL:HHC	23:BU:607:CHL:HBB1	1.96	0.47
2:6:44:ASN:OD1	2:6:204:VAL:HG13	2.14	0.47
3:8:176:THR:HA	3:8:178:TRP:CZ3	2.49	0.47
3:8:221:LEU:HG	3:8:225:LYS:HE2	1.97	0.47
3:8:229:ILE:HD11	3:8:233:ARG:NH2	2.30	0.47
24:8:302:CLA:HBC3	28:8:312:XAT:C12	2.44	0.47
24:B:605:CLA:H62	24:B:605:CLA:H41	1.51	0.47
24:B:608:CLA:H92	24:B:608:CLA:H62	1.72	0.47
8:N:76:GLY:HA3	8:N:216:LEU:HD23	1.95	0.47
10:i:14:PHE:O	10:i:18:LEU:HG	2.15	0.47
8:n:152:LEU:O	8:n:154:HIS:N	2.48	0.47
23:s:607:CHL:HBA2	23:s:607:CHL:H3A	1.49	0.47
2:0:230:GLN:HE22	24:0:613:CLA:CHA	2.28	0.47
23:0:601:CHL:H41	23:0:601:CHL:H61	1.52	0.47
3:AB:127:TRP:HE1	3:AB:252:PRO:CD	2.28	0.47
24:v:608:CLA:HBA2	24:v:608:CLA:H3A	1.54	0.47
24:BE:605:CLA:H193	24:BE:617:CLA:H201	1.97	0.47
24:BE:615:CLA:H11	24:BE:615:CLA:CHA	2.45	0.47
27:BE:624:LHG:H172	12:BO:20:TRP:HZ3	1.79	0.47
14:BV:131:PRO:HB3	14:BV:141:CYS:SG	2.54	0.47
21:1:209:ILE:HG22	21:1:210:PHE:HD2	1.79	0.47
38:BD:408:PHO:H141	38:BD:408:PHO:H161	1.64	0.47
21:BF:297:TYR:OH	24:BF:502:CLA:O1A	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BU:609:CLA:C4A	24:BU:609:CLA:H11	2.45	0.47
3:8:237:VAL:O	3:8:241:ILE:HG22	2.15	0.47
4:B:90:LEU:HG	4:B:91:TRP:CD1	2.50	0.47
4:B:243:ALA:HA	4:B:246:PHE:CD2	2.50	0.47
24:B:610:CLA:H13	24:B:612:CLA:H12	1.96	0.47
29:F:101:BCR:H20C	29:F:101:BCR:H361	1.78	0.47
8:G:94:ARG:HH12	8:N:82:THR:HA	1.79	0.47
8:G:130:VAL:HB	8:G:133:LYS:NZ	2.30	0.47
23:G:601:CHL:HBA1	23:G:601:CHL:H3A	1.56	0.47
23:G:608:CHL:H3A	23:G:608:CHL:HBA2	1.43	0.47
14:S:73:ASP:OD2	14:S:74:GLY:N	2.48	0.47
12:l:12:GLU:HA	13:m:29:THR:CG2	2.45	0.47
8:y:121:ARG:NH1	8:y:245:ALA:HB2	2.30	0.47
32:A:413:SQD:H291	32:A:413:SQD:H321	1.49	0.47
22:r:250:MET:HE2	24:r:602:CLA:HMC1	1.96	0.47
23:r:605:CHL:HBC2	23:r:606:CHL:HBC3	1.96	0.47
28:9:619:XAT:H12	27:0:617:LHG:H192	1.97	0.47
5:2:266:ARG:NH1	20:R:220:THR:HG23	2.29	0.47
14:A6:242:GLN:O	14:A6:246:THR:HG22	2.15	0.47
24:BE:606:CLA:HBB1	24:BE:607:CLA:H51	1.96	0.47
24:BE:607:CLA:H142	24:BE:607:CLA:H111	1.68	0.47
24:Ba:313:CLA:HMC3	25:Ba:316:LUT:H191	1.96	0.47
25:BU:615:LUT:C8	25:BU:615:LUT:H181	2.44	0.47
2:6:70:GLU:OE1	2:6:70:GLU:N	2.45	0.46
24:6:602:CLA:H3A	24:6:602:CLA:O2A	2.15	0.46
5:D:162:PRO:HB3	5:D:171:ALA:HB2	1.96	0.46
7:F:24:THR:O	7:F:28:LEU:HD23	2.15	0.46
8:N:151:SER:HB3	14:S:139:ALA:HB2	1.96	0.46
23:N:608:CHL:C9	23:N:608:CHL:C11	2.93	0.46
4:b:151:PHE:CE2	4:b:203:ILE:HG23	2.49	0.46
11:k:50:LEU:HA	11:k:53:VAL:HG12	1.97	0.46
14:s:131:PRO:HB3	14:s:141:CYS:SG	2.54	0.46
14:s:159:THR:OG1	14:s:166:ASN:OD1	2.32	0.46
20:A:183:MET:HE1	24:A:406:CLA:HMD1	1.96	0.46
1:9:152:LEU:O	1:9:154:HIS:N	2.49	0.46
24:9:613:CLA:HBB1	24:9:613:CLA:HMB1	1.97	0.46
8:Au:65:GLU:OE2	8:Au:66:SER:N	2.49	0.46
24:Au:613:CLA:H102	28:BB:301:XAT:H15	1.96	0.46
13:A1:8:PHE:C	13:A1:8:PHE:CD2	2.94	0.46
23:BB:306:CHL:HBA2	23:BB:306:CHL:H3A	1.46	0.46
24:BE:603:CLA:H151	24:BE:603:CLA:H18	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BV:602:CLA:H61	25:BV:615:LUT:H373	1.97	0.46
20:BD:183:MET:HE1	24:BD:406:CLA:HHD	1.97	0.46
23:BU:605:CHL:H193	23:BU:607:CHL:HBB2	1.95	0.46
1:5:134:ALA:O	1:5:137:GLN:HG2	2.15	0.46
28:5:619:XAT:O3	2:6:261:PHE:HB2	2.15	0.46
9:H:21:LYS:HA	9:H:24:LYS:HG2	1.97	0.46
23:N:605:CHL:HBA2	23:N:605:CHL:H3A	1.54	0.46
14:S:242:GLN:O	14:S:246:THR:HG22	2.15	0.46
8:Y:100:VAL:O	8:Y:103:SER:OG	2.26	0.46
8:Y:250:ASP:C	8:Y:250:ASP:OD1	2.58	0.46
4:b:151:PHE:CE2	4:b:207:THR:HG22	2.51	0.46
4:b:243:ALA:HA	4:b:246:PHE:CD2	2.49	0.46
4:b:458:PHE:HB3	24:b:605:CLA:HBC2	1.96	0.46
24:b:615:CLA:H11	24:b:615:CLA:CHA	2.45	0.46
5:d:349:ARG:HB2	5:d:353:LEU:HD12	1.97	0.46
20:a:202:VAL:HG11	24:a:407:CLA:OBD	2.16	0.46
38:a:408:PHO:H161	38:a:408:PHO:H141	1.64	0.46
22:r:158:GLU:OE1	22:r:267:PRO:HD2	2.15	0.46
22:r:254:LEU:O	22:r:258:VAL:HG12	2.16	0.46
22:r:284:ILE:O	22:r:288:SER:N	2.47	0.46
1:9:125:LYS:NZ	1:9:148:GLY:HA3	2.31	0.46
25:9:616:LUT:H181	25:9:616:LUT:H8	1.97	0.46
1:AA:121:ARG:HH22	1:AA:242:GLU:HA	1.81	0.46
5:2:233:PHE:CE2	32:2:408:SQD:H461	2.50	0.46
24:A2:603:CLA:H191	27:BB:319:LHG:H223	1.97	0.46
4:BE:41:GLU:HB3	4:BE:60:MET:CE	2.38	0.46
8:BJ:162:TRP:CE2	23:BJ:607:CHL:HBC2	2.51	0.46
24:BJ:602:CLA:H142	24:BJ:602:CLA:H111	1.81	0.46
23:BQ:608:CHL:H143	23:BQ:608:CHL:H162	1.78	0.46
14:BV:183:GLY:HA2	24:BV:608:CLA:HAB	1.97	0.46
24:BV:602:CLA:HBA2	24:BV:602:CLA:H3A	1.30	0.46
21:1:157:MET:HE2	21:1:271:TYR:HE2	1.80	0.46
20:BD:308:ASP:OD1	20:BD:312:ARG:N	2.39	0.46
1:5:105:TRP:NE1	23:5:608:CHL:HED3	2.30	0.46
1:7:161:ILE:HD12	1:7:161:ILE:H	1.80	0.46
5:D:197:PHE:HD1	5:D:282:MET:HG3	1.80	0.46
8:G:214:LYS:O	8:G:218:ASN:ND2	2.44	0.46
30:I:101:LMG:H122	34:A:402:DGD:HA32	1.97	0.46
24:I:102:CLA:H191	20:A:120:LEU:HB3	1.97	0.46
23:N:606:CHL:OMC	25:N:616:LUT:H163	2.15	0.46
25:N:615:LUT:H181	25:N:615:LUT:C8	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:168:LEU:O	8:n:172:VAL:HG23	2.15	0.46
24:n:603:CLA:H203	24:n:603:CLA:H162	1.74	0.46
26:s:616:NEX:H10	26:s:616:NEX:H181	1.98	0.46
8:y:169:MET:HA	8:y:172:VAL:HG22	1.96	0.46
20:A:308:ASP:OD1	20:A:312:ARG:N	2.40	0.46
21:C:209:ILE:HG22	21:C:210:PHE:HD1	1.81	0.46
21:C:344:SER:N	21:C:348:GLU:O	2.44	0.46
1:9:214:LYS:NZ	24:9:612:CLA:O1A	2.37	0.46
23:BB:307:CHL:HBD	23:BB:307:CHL:HAA1	1.97	0.46
23:BQ:607:CHL:H203	23:BQ:607:CHL:H161	1.72	0.46
14:BV:105:GLU:OE1	14:BV:105:GLU:N	2.48	0.46
23:Ba:302:CHL:H202	23:Ba:302:CHL:H161	1.69	0.46
32:R:411:SQD:H202	32:R:411:SQD:H172	1.62	0.46
21:BF:62:PHE:HB2	21:BF:122:SER:OG	2.15	0.46
1:7:121:ARG:HH22	1:7:242:GLU:HA	1.80	0.46
3:8:71:GLU:CD	3:8:71:GLU:H	2.24	0.46
5:D:224:PHE:CZ	5:D:246:SER:HB2	2.51	0.46
25:G:615:LUT:C8	25:G:615:LUT:H181	2.45	0.46
32:L:101:SQD:H142	32:l:101:SQD:H383	1.97	0.46
24:b:604:CLA:H143	24:b:604:CLA:H161	1.77	0.46
5:d:85:SER:HB2	16:u:102:ARG:NH2	2.30	0.46
5:d:158:PHE:C	5:d:159:LEU:HD23	2.41	0.46
24:C:513:CLA:HBD	24:C:513:CLA:HED3	1.78	0.46
21:c:223:TRP:CG	21:c:224:ILE:H	2.33	0.46
24:c:513:CLA:H161	24:c:514:CLA:H13	1.97	0.46
24:r:602:CLA:HBC1	27:r:618:LHG:H281	1.97	0.46
1:9:238:LYS:HD2	1:9:242:GLU:OE2	2.16	0.46
23:AA:308:CHL:H3A	23:AA:308:CHL:HBA1	1.61	0.46
3:AB:110:MET:O	3:AB:113:VAL:HG12	2.15	0.46
3:AB:225:LYS:O	3:AB:229:ILE:HG22	2.15	0.46
4:v:257:TRP:HB2	4:v:452:THR:HG21	1.98	0.46
4:BE:41:GLU:CD	4:BE:62:VAL:HG22	2.41	0.46
8:BQ:121:ARG:NH1	8:BQ:121:ARG:O	2.48	0.46
8:BQ:152:LEU:O	8:BQ:154:HIS:N	2.48	0.46
24:BQ:603:CLA:H203	24:BQ:603:CLA:H162	1.74	0.46
14:BV:242:GLN:O	14:BV:246:THR:HG22	2.15	0.46
8:Ba:155:ALA:HA	23:Ba:306:CHL:C1C	2.46	0.46
20:R:159:LEU:C	20:R:162:PRO:HD2	2.41	0.46
22:BU:250:MET:CE	24:BU:602:CLA:HAB	2.45	0.46
2:6:93:ARG:O	2:6:97:VAL:HG13	2.15	0.46
23:6:609:CHL:HHC	23:6:609:CHL:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:613:CLA:H8	24:6:613:CLA:H51	1.65	0.46
4:B:151:PHE:CD1	4:B:151:PHE:C	2.92	0.46
5:D:322:LEU:HD13	20:A:184:ILE:HG21	1.97	0.46
24:Y:303:CLA:H12	24:Y:303:CLA:H3A	1.98	0.46
19:Z:14:ILE:O	19:Z:18:ILE:HG22	2.15	0.46
23:g:607:CHL:CBB	25:g:616:LUT:H193	2.44	0.46
34:h:102:DGD:HB91	34:h:102:DGD:HB62	1.69	0.46
24:n:610:CLA:HBB1	24:n:610:CLA:HMB3	1.96	0.46
24:y:303:CLA:H141	24:y:303:CLA:H161	1.73	0.46
24:y:304:CLA:HHC	24:y:304:CLA:HBB1	1.98	0.46
23:y:306:CHL:HBA2	23:y:306:CHL:H3A	1.56	0.46
20:a:248:ILE:HD12	20:a:248:ILE:H	1.80	0.46
23:r:605:CHL:HBA2	26:r:617:NEX:H28	1.97	0.46
24:r:609:CLA:C4A	24:r:609:CLA:H11	2.45	0.46
1:9:105:TRP:NE1	23:9:608:CHL:HED3	2.29	0.46
1:9:231:VAL:HG11	24:9:613:CLA:CAC	2.46	0.46
32:2:408:SQD:H111	32:2:408:SQD:H142	1.50	0.46
7:4:17:VAL:HG23	7:4:18:HIS:HD1	1.81	0.46
12:Az:13:LEU:HD21	13:A1:26:TYR:CA	2.44	0.46
8:A2:152:LEU:O	8:A2:154:HIS:N	2.47	0.46
4:BE:468:TRP:HE1	4:BE:472:ARG:HH21	1.63	0.46
24:BE:610:CLA:C4D	9:BK:43:MET:HE1	2.45	0.46
23:BJ:608:CHL:H3A	23:BJ:608:CHL:HBA2	1.42	0.46
9:BK:56:ILE:O	9:BK:60:ILE:HG12	2.16	0.46
20:BD:248:ILE:H	20:BD:248:ILE:HD12	1.79	0.46
21:BF:365:TRP:CD1	21:BF:365:TRP:H	2.33	0.46
24:BF:509:CLA:H141	24:BF:509:CLA:H161	1.71	0.46
2:6:170:VAL:HA	2:6:173:PHE:HD1	1.79	0.46
5:D:321:LEU:O	20:A:331:MET:HE2	2.15	0.46
9:H:47:MET:HE1	29:H:101:BCR:HC8	1.97	0.46
29:H:101:BCR:H24C	29:H:101:BCR:H371	1.80	0.46
16:U:82:GLU:O	16:U:86:LYS:HG2	2.14	0.46
23:Y:307:CHL:HAA1	23:Y:307:CHL:HBD	1.97	0.46
4:b:170:ASP:OD2	4:b:175:THR:N	2.44	0.46
24:s:602:CLA:H61	25:s:615:LUT:H373	1.98	0.46
23:s:606:CHL:C9	23:s:606:CHL:C11	2.93	0.46
8:y:214:LYS:HE3	8:y:214:LYS:HB2	1.75	0.46
23:y:302:CHL:H41	23:y:302:CHL:H61	1.68	0.46
29:A:411:BCR:H24C	29:A:411:BCR:H371	1.78	0.46
1:AA:186:ALA:HB2	23:AA:309:CHL:HBC1	1.97	0.46
23:Au:601:CHL:H3A	23:Au:601:CHL:HBA1	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BJ:606:CHL:HBB2	23:BJ:607:CHL:CBB	2.46	0.46
23:BV:605:CHL:HMC	23:BV:606:CHL:NC	2.31	0.46
20:R:184:ILE:O	20:R:328:MET:HE1	2.16	0.46
21:BF:71:GLU:HB3	21:BF:89:LEU:HD13	1.98	0.46
24:BF:505:CLA:H11	34:BF:518:DGD:HB42	1.97	0.46
24:BF:513:CLA:H161	24:BF:514:CLA:H13	1.98	0.46
22:BU:254:LEU:O	22:BU:258:VAL:HG12	2.16	0.46
1:5:126:PHE:CE1	1:5:147:LEU:HA	2.51	0.46
2:6:163:GLN:HE22	23:6:607:CHL:HMC	1.80	0.46
2:6:221:MET:HE3	25:6:616:LUT:C34	2.46	0.46
1:7:241:LEU:O	1:7:244:LEU:HG	2.15	0.46
24:B:606:CLA:H72	29:B:619:BCR:H321	1.98	0.46
5:D:78:ALA:HB2	5:D:175:GLY:HA3	1.97	0.46
27:D:404:LHG:H281	15:T:17:ILE:HD11	1.98	0.46
10:I:27:ASP:OD2	21:C:449:ARG:NH1	2.43	0.46
14:S:233:MET:HE1	24:S:602:CLA:HAB	1.96	0.46
14:s:183:GLY:HA2	24:s:608:CLA:HAB	1.98	0.46
19:z:61:ILE:HG13	19:z:62:SER:N	2.31	0.46
24:C:505:CLA:HBA2	24:C:505:CLA:H3A	1.56	0.46
20:a:140:ARG:HB3	20:a:142:TRP:CE3	2.50	0.46
21:c:162:GLY:HA3	21:c:252:ILE:HG13	1.98	0.46
22:r:283:ILE:HG12	23:r:613:CHL:HED1	1.97	0.46
2:0:93:ARG:O	2:0:97:VAL:HG13	2.15	0.46
2:0:150:LEU:O	2:0:152:HIS:N	2.49	0.46
23:0:607:CHL:H3A	23:0:607:CHL:HBA1	1.41	0.46
3:AB:83:PHE:CE2	28:AB:312:XAT:H242	2.50	0.46
4:v:419:LYS:NZ	4:v:420:TYR:CE1	2.83	0.46
5:2:137:VAL:CG2	5:2:139:LEU:HD23	2.42	0.46
30:Aw:101:LMG:H122	34:R:401:DGD:HA32	1.98	0.46
25:A2:615:LUT:C8	25:A2:615:LUT:H181	2.46	0.46
23:A6:607:CHL:H3A	23:A6:607:CHL:HBA2	1.50	0.46
15:A7:17:ILE:O	15:A7:21:ILE:HG22	2.16	0.46
4:BE:234:ILE:O	4:BE:237:VAL:HG22	2.16	0.46
22:BU:155:LEU:HD12	22:BU:155:LEU:HA	1.74	0.46
23:BU:613:CHL:HHC	23:BU:613:CHL:HBB1	1.98	0.46
23:N:601:CHL:H62	23:N:601:CHL:H41	1.68	0.46
24:N:603:CLA:H191	27:Y:319:LHG:H223	1.97	0.46
24:N:610:CLA:HBA2	24:N:610:CLA:H12	1.53	0.46
19:Z:1:MET:SD	19:Z:1:MET:C	2.98	0.46
4:b:231:MET:CE	24:b:611:CLA:HMC1	2.46	0.46
29:b:618:BCR:H15C	29:b:618:BCR:H351	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g:601:CHL:HED3	24:g:602:CLA:HBC1	1.97	0.46
32:a:412:SQD:H202	32:a:412:SQD:H172	1.77	0.46
23:r:613:CHL:HHC	23:r:613:CHL:HBB1	1.98	0.46
1:AA:183:LEU:HG	23:AA:309:CHL:HBB1	1.97	0.46
24:AB:303:CLA:HBA2	24:AB:303:CLA:H3A	1.52	0.46
29:v:619:BCR:H371	29:v:619:BCR:H24C	1.77	0.46
5:2:344:GLU:OE1	5:2:344:GLU:N	2.49	0.46
24:Au:611:CLA:H51	24:Au:612:CLA:C3D	2.45	0.46
11:Ay:40:MET:HA	11:Ay:43:ILE:HG12	1.98	0.46
24:A6:604:CLA:CHA	24:A6:604:CLA:HBA1	2.46	0.46
24:A6:609:CLA:H3A	24:A6:609:CLA:CGA	2.46	0.46
4:BE:25:MET:HE1	29:BE:618:BCR:H393	1.98	0.46
4:BE:91:TRP:CE3	24:BE:607:CLA:HBD	2.51	0.46
24:BQ:610:CLA:HBB1	24:BQ:612:CLA:HAA1	1.97	0.46
24:BQ:610:CLA:H42	25:BQ:615:LUT:H26	1.97	0.46
14:BV:189:ARG:NH2	24:BV:608:CLA:O1D	2.49	0.46
8:Ba:121:ARG:NH1	8:Ba:245:ALA:HB2	2.30	0.46
8:Ba:128:GLU:H	8:Ba:137:GLN:HE22	1.64	0.46
20:R:218:LEU:HD11	20:R:251:ALA:HB1	1.98	0.46
34:BD:401:DGD:HB71	34:BD:401:DGD:HBT2	1.71	0.46
1:5:100:VAL:HG11	1:5:190:LEU:HG	1.98	0.46
1:5:105:TRP:CD1	23:5:609:CHL:HMD2	2.51	0.46
1:5:236:THR:HB	1:5:238:LYS:NZ	2.31	0.46
2:6:167:MET:HE1	23:6:609:CHL:C1C	2.46	0.46
24:B:614:CLA:H112	24:B:614:CLA:H91	1.70	0.46
4:b:324:LEU:HA	5:d:294:LEU:HD12	1.98	0.46
24:b:614:CLA:H41	24:b:614:CLA:H61	1.46	0.46
24:c:514:CLA:H92	27:c:520:LHG:H122	1.97	0.46
22:r:231:ASP:OD2	22:r:233:GLU:HG3	2.16	0.46
24:r:604:CLA:C1B	26:r:617:NEX:H383	2.45	0.46
25:r:615:LUT:H161	25:r:615:LUT:H7	1.78	0.46
2:0:44:ASN:OD1	2:0:204:VAL:HG13	2.16	0.46
23:0:606:CHL:HAA1	23:0:606:CHL:HBD	1.97	0.46
4:v:164:PRO:HG3	24:v:606:CLA:O1D	2.16	0.46
4:v:296:GLN:OE1	4:v:296:GLN:N	2.49	0.46
24:v:614:CLA:H112	24:v:614:CLA:H91	1.70	0.46
24:v:614:CLA:HMB1	24:v:614:CLA:HBB1	1.96	0.46
8:BB:229:PHE:HE1	25:BB:316:LUT:H41	1.80	0.46
4:BE:472:ARG:HG3	4:BE:479:PHE:CE2	2.50	0.46
20:R:289:GLY:O	20:R:293:MET:HG2	2.15	0.46
21:1:269:GLU:OE2	21:1:444:HIS:ND1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BD:268:SER:O	20:BD:271:LEU:HG	2.16	0.46
21:BF:148:GLY:O	21:BF:156:LYS:NZ	2.46	0.46
22:BU:148:MET:HE3	22:BU:149:LEU:N	2.31	0.46
2:6:112:THR:O	2:6:116:LEU:HG	2.16	0.46
3:8:83:PHE:CE2	28:8:312:XAT:H242	2.51	0.46
3:8:203:LEU:HD23	25:8:311:LUT:H222	1.98	0.46
8:G:171:ALA:HB1	8:G:175:TYR:HE1	1.81	0.46
12:L:22:LEU:HB3	15:T:16:ILE:HD13	1.97	0.46
17:W:131:LEU:HD22	21:C:452:ALA:HB1	1.98	0.46
8:Y:65:GLU:OE2	8:Y:65:GLU:N	2.40	0.46
24:b:614:CLA:H111	24:b:614:CLA:H91	1.65	0.46
5:d:25:ARG:HB3	5:d:27:ARG:NH2	2.31	0.46
8:y:128:GLU:H	8:y:137:GLN:HE22	1.64	0.46
23:y:302:CHL:H41	27:y:319:LHG:H192	1.97	0.46
21:c:297:TYR:OH	24:c:502:CLA:O1A	2.29	0.46
1:AA:67:PRO:HD2	1:AA:70:LEU:HD12	1.98	0.46
1:AA:223:MET:CE	24:AA:303:CLA:HMC3	2.45	0.46
4:v:132:SER:HB2	9:Av:30:TYR:CD1	2.51	0.46
24:v:609:CLA:H62	24:v:609:CLA:H41	1.76	0.46
8:A2:202:ALA:HB2	24:A2:610:CLA:HAA2	1.98	0.46
23:A2:601:CHL:H62	23:A2:601:CHL:H41	1.66	0.46
14:A6:182:LEU:HD12	14:A6:182:LEU:HA	1.72	0.46
16:A8:80:GLY:HA3	16:A8:103:TYR:HB3	1.98	0.46
8:BB:117:GLU:OE1	8:BB:121:ARG:HG3	2.15	0.46
23:BB:302:CHL:H3A	23:BB:302:CHL:HBA1	1.45	0.46
14:BV:122:MET:HE3	14:BV:229:GLY:N	2.31	0.46
8:Ba:207:ALA:O	8:Ba:211:LEU:HG	2.15	0.46
21:1:307:PRO:HB3	21:1:358:PHE:HB3	1.98	0.46
20:BD:297:LEU:HD12	20:BD:297:LEU:HA	1.78	0.46
32:BD:412:SQD:H321	32:BD:412:SQD:H291	1.54	0.46
24:BF:502:CLA:HHC	24:BF:502:CLA:HBB1	1.98	0.46
24:5:613:CLA:HMB1	24:5:613:CLA:HBB1	1.97	0.45
24:8:308:CLA:H3A	24:8:308:CLA:HBA2	1.52	0.45
4:B:216:HIS:CE1	24:B:609:CLA:C1A	2.98	0.45
4:B:366:PHE:CD1	4:B:367:PRO:HD2	2.51	0.45
24:B:602:CLA:H91	24:B:602:CLA:H111	1.72	0.45
14:S:67:ARG:HE	14:S:92:ASP:CG	2.24	0.45
15:T:17:ILE:HD12	15:T:17:ILE:HA	1.86	0.45
4:b:91:TRP:CE3	24:b:607:CLA:HBD	2.51	0.45
5:d:202:VAL:HG22	24:d:401:CLA:C2B	2.46	0.45
8:g:173:GLU:HB3	23:g:609:CHL:HHB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:219:GLY:O	8:n:223:MET:HE2	2.16	0.45
19:z:57:LEU:O	19:z:61:ILE:HG23	2.16	0.45
24:A:405:CLA:H72	24:A:405:CLA:H111	1.80	0.45
24:c:508:CLA:H202	24:c:508:CLA:H161	1.67	0.45
1:9:178:ALA:HA	2:0:62:GLN:HE22	1.80	0.45
2:0:167:MET:HE3	2:0:167:MET:HB3	1.56	0.45
3:AB:230:LYS:HE3	24:AB:309:CLA:C3D	2.46	0.45
24:AB:303:CLA:C4B	29:AB:313:BCR:H281	2.45	0.45
13:A1:8:PHE:C	13:A1:8:PHE:HD2	2.24	0.45
24:A2:602:CLA:H93	24:A2:602:CLA:H111	1.71	0.45
24:A2:611:CLA:H61	24:A2:611:CLA:H41	1.78	0.45
14:A6:197:GLU:H	14:A6:197:GLU:CD	2.24	0.45
31:BG:403:PL9:H501	20:BD:49:ILE:HG12	1.98	0.45
25:BJ:616:LUT:C8	25:BJ:616:LUT:H181	2.46	0.45
23:Ba:307:CHL:HAA1	23:Ba:307:CHL:CGD	2.45	0.45
20:R:328:MET:HE2	20:R:328:MET:HB3	1.71	0.45
21:BF:254:THR:C	21:BF:255:LYS:HD3	2.41	0.45
22:BU:233:GLU:O	22:BU:237:GLN:HG2	2.16	0.45
1:5:180:ASP:OD1	1:5:181:GLY:N	2.49	0.45
4:B:98:GLY:O	4:B:102:VAL:HG22	2.16	0.45
24:B:609:CLA:H92	24:B:609:CLA:H61	1.76	0.45
8:N:152:LEU:O	8:N:154:HIS:N	2.49	0.45
8:N:186:ALA:HB2	23:N:608:CHL:HBC1	1.98	0.45
23:N:608:CHL:H51	23:N:608:CHL:H12	1.66	0.45
25:Y:317:LUT:H181	25:Y:317:LUT:C8	2.46	0.45
8:n:169:MET:SD	23:n:609:CHL:C1C	3.04	0.45
23:n:608:CHL:H12	23:n:608:CHL:H51	1.66	0.45
17:w:117:PHE:HA	17:w:120:THR:HG22	1.96	0.45
19:z:46:LEU:O	19:z:50:LEU:HD23	2.17	0.45
22:r:127:TYR:OH	22:r:215:ARG:HD3	2.16	0.45
1:9:119:LEU:HD12	1:9:124:VAL:HG21	1.98	0.45
1:9:201:LEU:HD12	24:9:610:CLA:H11	1.98	0.45
2:0:111:ILE:HD12	2:0:111:ILE:HA	1.85	0.45
1:AA:230:PHE:C	1:AA:230:PHE:CD2	2.92	0.45
3:AB:114:LEU:HD23	3:AB:114:LEU:O	2.16	0.45
4:v:25:MET:HE1	4:v:108:PHE:HD1	1.81	0.45
5:2:108:LEU:CD2	6:3:76:LEU:HD11	2.47	0.45
8:Au:130:VAL:HB	8:Au:133:LYS:NZ	2.31	0.45
8:BB:223:MET:HE2	24:BB:303:CLA:HMC2	1.99	0.45
23:BB:308:CHL:C9	23:BB:308:CHL:C11	2.94	0.45
4:BE:134:ASP:OD1	9:BK:30:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BE:608:CLA:H92	24:BE:608:CLA:H62	1.70	0.45
5:BG:85:SER:HB2	16:BX:102:ARG:NH2	2.31	0.45
5:BG:272:MET:HE3	5:BG:272:MET:HB2	1.75	0.45
7:BI:31:ILE:O	7:BI:35:GLN:NE2	2.41	0.45
13:BP:1:MET:SD	13:BP:2:GLU:N	2.89	0.45
8:BQ:169:MET:SD	23:BQ:609:CHL:C2C	3.04	0.45
14:BV:241:ILE:HG21	24:BV:612:CLA:HAC2	1.96	0.45
23:BV:601:CHL:HBB1	23:BV:601:CHL:CHC	2.46	0.45
23:BV:606:CHL:C9	23:BV:606:CHL:C11	2.94	0.45
29:1:515:BCR:H15C	29:1:515:BCR:H351	1.83	0.45
23:6:601:CHL:H3A	23:6:601:CHL:HBA1	1.50	0.45
1:7:92:PHE:O	1:7:96:ARG:HG2	2.16	0.45
3:8:170:GLN:HG3	23:8:306:CHL:HMC	1.97	0.45
4:B:54:PRO:HD2	4:B:57:ARG:HG3	1.97	0.45
24:B:603:CLA:H193	24:B:603:CLA:H162	1.79	0.45
24:B:604:CLA:H193	24:B:616:CLA:H201	1.98	0.45
17:W:125:GLU:OE1	17:W:125:GLU:N	2.48	0.45
7:f:27:PHE:HE2	29:f:101:BCR:H12C	1.82	0.45
8:g:219:GLY:O	8:g:223:MET:HG3	2.16	0.45
25:g:616:LUT:H181	25:g:616:LUT:C8	2.46	0.45
8:y:119:LEU:HD12	8:y:124:VAL:HG21	1.98	0.45
24:y:313:CLA:HHC	24:y:313:CLA:HBB1	1.99	0.45
21:c:71:GLU:CD	21:c:86:LEU:HB3	2.41	0.45
24:r:609:CLA:H193	24:r:609:CLA:H161	1.74	0.45
1:9:221:LEU:HD11	24:9:611:CLA:HAC2	1.99	0.45
5:2:162:PRO:HB3	5:2:171:ALA:HB2	1.97	0.45
23:Au:601:CHL:HED1	27:Au:618:LHG:H122	1.98	0.45
23:A2:608:CHL:HAB	26:A2:617:NEX:H202	1.98	0.45
23:BB:307:CHL:HAA1	23:BB:307:CHL:CBD	2.46	0.45
4:BE:221:PRO:O	9:BK:33:VAL:HG23	2.17	0.45
4:BE:223:GLN:CD	4:BE:223:GLN:H	2.24	0.45
6:BH:78:GLU:OE1	6:BH:81:ARG:NH1	2.50	0.45
24:BJ:610:CLA:HBA2	24:BJ:610:CLA:H3A	1.33	0.45
12:BO:34:ASN:OD1	12:BO:34:ASN:N	2.50	0.45
21:1:319:VAL:O	21:1:322:GLN:HG3	2.16	0.45
21:1:433:LEU:HD23	24:1:503:CLA:HMC2	1.98	0.45
2:6:147:ASN:HB3	2:6:150:LEU:HG	1.98	0.45
4:B:257:TRP:HB2	4:B:452:THR:HG21	1.97	0.45
23:G:606:CHL:HMC	25:G:616:LUT:H163	1.98	0.45
24:I:102:CLA:H192	24:I:102:CLA:H161	1.78	0.45
23:Y:308:CHL:HAA1	23:Y:308:CHL:HBD	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:45:PHE:HB2	4:b:60:MET:HE3	1.99	0.45
5:d:28:PHE:CG	5:d:29:VAL:N	2.84	0.45
5:d:68:TYR:O	7:f:34:MET:HE2	2.17	0.45
14:s:100:LEU:HA	2:0:178:LEU:HD22	1.97	0.45
23:s:601:CHL:HBB1	23:s:601:CHL:CHC	2.45	0.45
24:s:608:CLA:H3A	24:s:608:CLA:HBA2	1.63	0.45
24:s:609:CLA:H2	25:s:614:LUT:H28	1.96	0.45
15:t:1:MET:SD	15:t:2:GLU:N	2.89	0.45
24:A:407:CLA:O1A	24:A:407:CLA:H3A	2.17	0.45
22:r:132:GLY:O	22:r:135:ARG:HB2	2.16	0.45
1:9:188:ASP:OD1	1:9:191:TYR:N	2.42	0.45
2:0:163:GLN:NE2	23:0:607:CHL:HMC	2.32	0.45
24:AA:303:CLA:CBB	25:AA:317:LUT:H32	2.46	0.45
24:AA:303:CLA:HBB2	25:AA:317:LUT:H32	1.97	0.45
3:AB:162:VAL:HG21	22:BU:59:TYR:OH	2.16	0.45
26:BB:320:NEX:H383	24:BU:604:CLA:C1B	2.46	0.45
19:BC:5:PHE:O	19:BC:9:VAL:HG13	2.17	0.45
4:BE:243:ALA:HA	4:BE:246:PHE:CD2	2.51	0.45
24:BE:612:CLA:H2A	24:BE:612:CLA:HED2	1.98	0.45
23:BJ:601:CHL:H62	23:BJ:601:CHL:H41	1.73	0.45
29:BN:101:BCR:HC42	29:Bb:101:BCR:H343	1.99	0.45
14:BV:207:ASP:OD1	24:BV:609:CLA:HBD	2.17	0.45
20:R:88:ALA:HA	21:1:356:MET:HE1	1.98	0.45
24:R:404:CLA:H72	24:R:405:CLA:HBB1	1.99	0.45
21:1:396:MET:HG3	21:1:397:THR:N	2.32	0.45
24:1:504:CLA:H172	24:1:510:CLA:HBB2	1.98	0.45
24:BF:507:CLA:H12	29:BF:516:BCR:H321	1.98	0.45
2:6:112:THR:O	2:6:115:VAL:HG22	2.17	0.45
24:7:312:CLA:C4D	24:7:313:CLA:HMD3	2.47	0.45
7:F:31:ILE:O	7:F:34:MET:HG3	2.17	0.45
12:L:13:LEU:HD21	13:M:26:TYR:CA	2.43	0.45
23:Y:307:CHL:HAA1	23:Y:307:CHL:CBD	2.46	0.45
24:b:603:CLA:H151	24:b:603:CLA:H18	1.84	0.45
24:b:610:CLA:C4D	9:h:43:MET:HE1	2.46	0.45
5:d:200:MET:CE	31:d:403:PL9:H272	2.45	0.45
11:k:43:ILE:HA	11:k:46:PHE:HD1	1.82	0.45
21:C:321:ASP:OD2	21:C:340:TYR:OH	2.25	0.45
20:a:204:GLY:HA2	20:a:278:TRP:NE1	2.32	0.45
24:c:508:CLA:H93	24:c:508:CLA:H112	1.79	0.45
34:c:517:DGD:HB31	30:c:518:LMG:H321	1.97	0.45
1:9:176:ARG:NH1	23:9:609:CHL:HED1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:92:PHE:O	1:AA:96:ARG:HG2	2.17	0.45
4:v:42:LEU:HD23	4:v:42:LEU:HA	1.70	0.45
24:v:610:CLA:H13	24:v:612:CLA:H12	1.97	0.45
5:2:266:ARG:NE	5:2:266:ARG:CA	2.79	0.45
8:Au:93:ALA:O	8:Au:97:GLU:HG2	2.16	0.45
25:Au:615:LUT:C8	25:Au:615:LUT:H181	2.45	0.45
13:A1:23:LEU:O	13:A1:27:VAL:HG23	2.16	0.45
8:A2:176:ARG:NH2	23:A2:609:CHL:O1D	2.41	0.45
19:BC:31:ASP:OD1	19:BC:34:SER:HB3	2.17	0.45
24:BE:609:CLA:CAB	5:BG:124:ILE:CD1	2.94	0.45
5:BG:183:ILE:HG23	24:BG:401:CLA:HAC1	1.97	0.45
9:BK:60:ILE:HA	9:BK:65:VAL:HG12	1.97	0.45
8:BQ:168:LEU:O	8:BQ:172:VAL:HG23	2.17	0.45
14:BV:72:PRO:HD3	23:BV:601:CHL:HHC	1.98	0.45
8:Ba:169:MET:HA	8:Ba:172:VAL:HG22	1.98	0.45
20:R:183:MET:HE1	24:R:405:CLA:HMD1	1.99	0.45
34:1:516:DGD:O4E	34:1:516:DGD:O5E	2.30	0.45
20:BD:289:GLY:O	20:BD:293:MET:HE3	2.16	0.45
21:BF:152:LYS:NZ	21:BF:152:LYS:HB3	2.31	0.45
2:6:239:LEU:HD12	2:6:239:LEU:HA	1.80	0.45
1:7:183:LEU:HG	23:7:309:CHL:HBB1	1.97	0.45
3:8:236:MET:HE3	24:8:301:CLA:CMC	2.46	0.45
29:B:623:BCR:H313	15:t:17:ILE:HG22	1.98	0.45
8:G:85:LEU:HB2	24:G:602:CLA:H11	1.98	0.45
8:G:247:HIS:CG	24:G:613:CLA:HAA2	2.52	0.45
13:M:23:LEU:O	13:M:27:VAL:HG23	2.17	0.45
8:N:105:TRP:CD1	23:N:609:CHL:HMD2	2.52	0.45
28:N:619:XAT:H203	24:Y:314:CLA:H72	1.99	0.45
24:Y:312:CLA:H91	24:Y:312:CLA:H111	1.77	0.45
4:b:367:PRO:HB2	5:d:346:VAL:HG11	1.98	0.45
8:n:227:PHE:O	8:n:231:VAL:HG12	2.16	0.45
23:n:607:CHL:H203	23:n:607:CHL:H161	1.71	0.45
14:s:174:ALA:O	14:s:178:GLU:HG3	2.17	0.45
20:A:159:LEU:C	20:A:162:PRO:HD2	2.42	0.45
30:A:412:LMG:H341	30:A:412:LMG:H372	1.72	0.45
22:r:159:TRP:HD1	22:r:160:LEU:CD2	2.25	0.45
22:r:250:MET:CE	24:r:602:CLA:HAB	2.45	0.45
22:r:253:PHE:CD2	28:r:616:XAT:H12	2.52	0.45
1:9:180:ASP:OD1	1:9:181:GLY:N	2.49	0.45
1:9:234:ILE:HA	1:9:234:ILE:HD12	1.82	0.45
2:0:221:MET:HB2	2:0:221:MET:HE3	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:74:PHE:HB3	1:AA:96:ARG:CZ	2.47	0.45
3:AB:162:VAL:HG11	22:BU:59:TYR:OH	2.17	0.45
3:AB:176:THR:HA	3:AB:178:TRP:CZ3	2.52	0.45
3:AB:236:MET:HE3	24:AB:301:CLA:CMC	2.47	0.45
4:v:25:MET:HE1	4:v:108:PHE:CD1	2.52	0.45
15:A7:15:GLY:HA2	29:BE:601:BCR:H12C	1.97	0.45
23:BB:308:CHL:C9	23:BB:308:CHL:H111	2.46	0.45
23:BB:308:CHL:HBD	23:BB:308:CHL:HAA1	1.99	0.45
4:BE:367:PRO:HB2	5:BG:346:VAL:CG1	2.47	0.45
13:BP:8:PHE:O	13:BP:11:THR:HG22	2.16	0.45
26:BV:616:NEX:C10	26:BV:616:NEX:H181	2.47	0.45
20:BD:183:MET:HB3	24:BD:405:CLA:HBC2	1.98	0.45
23:Y:308:CHL:C9	23:Y:308:CHL:C11	2.94	0.45
23:Y:308:CHL:C9	23:Y:308:CHL:H111	2.46	0.45
25:Y:316:LUT:H181	25:Y:316:LUT:C8	2.45	0.45
24:b:603:CLA:H171	34:h:102:DGD:HAW1	1.99	0.45
24:b:603:CLA:H91	24:b:603:CLA:H111	1.70	0.45
9:h:66:LEU:HD22	18:x:81:PRO:HG3	1.99	0.45
8:y:155:ALA:HA	23:y:306:CHL:C1C	2.46	0.45
2:0:75:TYR:OH	27:0:617:LHG:O5	2.26	0.45
24:0:613:CLA:C1D	24:0:613:CLA:H52	2.46	0.45
4:v:74:SER:HA	4:v:92:SER:HB2	1.98	0.45
25:BB:317:LUT:C8	25:BB:317:LUT:H181	2.47	0.45
24:BE:603:CLA:H91	24:BE:603:CLA:H111	1.67	0.45
5:BG:124:ILE:O	5:BG:128:LEU:HD22	2.16	0.45
8:BQ:103:SER:HB2	8:BQ:219:GLY:HA3	1.98	0.45
14:BV:144:GLU:OE2	14:BV:146:VAL:HB	2.16	0.45
23:BU:605:CHL:HMC	23:BU:606:CHL:C3C	2.47	0.45
1:5:186:ALA:HB2	23:5:608:CHL:HBC1	1.99	0.45
1:7:61:PRO:HD2	23:7:302:CHL:CBB	2.46	0.45
3:8:164:PHE:CD1	3:8:164:PHE:C	2.95	0.45
3:8:236:MET:HE3	24:8:301:CLA:HMC2	1.99	0.45
4:B:63:ILE:N	4:B:64:PRO:HD2	2.32	0.45
4:B:371:VAL:HG12	4:B:377:VAL:HA	1.99	0.45
24:B:612:CLA:H61	24:B:612:CLA:H102	1.64	0.45
24:B:614:CLA:H141	24:B:614:CLA:H161	1.62	0.45
24:B:615:CLA:H41	24:B:615:CLA:H61	1.54	0.45
8:G:65:GLU:OE2	8:G:66:SER:N	2.49	0.45
23:N:609:CHL:H193	23:N:609:CHL:H162	1.71	0.45
24:S:604:CLA:C1C	26:S:616:NEX:H222	2.47	0.45
5:d:252:ARG:CZ	21:c:469:MET:HE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:78:GLU:OE1	6:e:81:ARG:NH1	2.49	0.45
24:g:602:CLA:H3A	24:g:602:CLA:HBA2	1.49	0.45
17:w:110:GLY:HA3	27:w:201:LHG:H181	1.99	0.45
29:z:102:BCR:H361	29:z:102:BCR:H20C	1.84	0.45
25:9:615:LUT:H11	25:9:615:LUT:H191	1.84	0.45
2:0:224:MET:HA	2:0:224:MET:CE	2.42	0.45
3:AB:220:LYS:O	3:AB:224:LEU:HG	2.16	0.45
24:v:606:CLA:H111	24:v:606:CLA:H142	1.70	0.45
23:Au:607:CHL:HBB2	23:Au:609:CHL:HBC1	1.99	0.45
8:A2:105:TRP:CD1	23:A2:609:CHL:HMD2	2.52	0.45
26:BB:320:NEX:H403	23:BU:605:CHL:HBA1	1.99	0.45
4:BE:121:GLU:CD	9:BK:14:PRO:HB2	2.42	0.45
4:BE:216:HIS:CE1	24:BE:610:CLA:C1A	2.99	0.45
4:BE:458:PHE:HB3	24:BE:605:CLA:HBC2	1.98	0.45
5:BG:54:THR:HA	5:BG:68:TYR:HD1	1.82	0.45
5:BG:156:SER:HA	5:BG:160:ILE:CD1	2.46	0.45
5:BG:297:TYR:OH	5:BG:327:ARG:NH1	2.45	0.45
5:BG:324:GLU:HG2	5:BG:327:ARG:NH2	2.31	0.45
34:BK:102:DGD:O4D	34:BK:102:DGD:O5D	2.34	0.45
8:Ba:175:TYR:CE1	8:Ba:182:PRO:HD3	2.52	0.45
8:Ba:214:LYS:HB2	8:Ba:214:LYS:HE3	1.75	0.45
24:R:406:CLA:O1A	24:R:406:CLA:H3A	2.17	0.45
20:BD:198:HIS:O	20:BD:202:VAL:HG13	2.16	0.45
1:7:186:ALA:HB2	23:7:309:CHL:HBC1	1.97	0.45
23:7:309:CHL:HBA2	23:7:309:CHL:H3A	1.48	0.45
3:8:230:LYS:HE3	24:8:309:CLA:C3D	2.47	0.45
29:B:619:BCR:H24C	29:B:619:BCR:H371	1.79	0.45
23:N:608:CHL:HAB	26:N:617:NEX:H202	1.98	0.45
8:Y:98:LEU:HD23	23:Y:310:CHL:HED3	1.98	0.45
23:Y:310:CHL:H143	23:Y:310:CHL:H162	1.87	0.45
24:b:611:CLA:H13	24:b:613:CLA:H12	1.99	0.45
23:n:606:CHL:CBB	25:n:616:LUT:H161	2.47	0.45
24:n:610:CLA:H62	24:n:612:CLA:CBA	2.44	0.45
14:s:144:GLU:OE2	14:s:146:VAL:HB	2.17	0.45
21:C:342:MET:HG2	21:C:352:GLY:HA2	1.99	0.45
20:a:225:ARG:HA	20:a:225:ARG:HD3	1.88	0.45
22:r:80:PRO:HG2	22:r:81:PHE:HD1	1.82	0.45
24:0:604:CLA:HBA2	24:0:604:CLA:H3A	1.30	0.45
32:A1:101:SQD:H342	32:A1:101:SQD:H312	1.51	0.45
24:BE:611:CLA:H102	24:BE:616:CLA:HAA1	1.98	0.45
24:BE:613:CLA:H102	24:BE:613:CLA:H61	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BE:614:CLA:H91	24:BE:614:CLA:H111	1.64	0.45
5:BG:265:LYS:HE3	20:BD:245:THR:HG22	1.98	0.45
7:BI:27:PHE:HE2	29:BI:101:BCR:H12C	1.81	0.45
24:Ba:304:CLA:HHC	24:Ba:304:CLA:HBB1	1.98	0.45
24:B:604:CLA:H203	27:B:621:LHG:H341	1.98	0.45
24:B:611:CLA:HMB1	24:B:611:CLA:HBB1	1.98	0.45
7:F:17:VAL:HG23	7:F:18:HIS:HD1	1.81	0.45
8:Y:90:GLU:OE1	8:Y:90:GLU:N	2.39	0.45
23:Y:307:CHL:HMC	23:Y:308:CHL:C4C	2.47	0.45
5:d:55:PHE:HD1	6:e:47:PHE:HE1	1.65	0.45
5:d:75:LEU:H	5:d:75:LEU:HD12	1.82	0.45
8:g:105:TRP:CD1	23:g:609:CHL:HMD3	2.51	0.45
12:l:34:ASN:OD1	12:l:34:ASN:N	2.50	0.45
23:s:605:CHL:OMC	25:s:615:LUT:H163	2.17	0.45
23:y:308:CHL:H111	23:y:308:CHL:H143	1.78	0.45
21:C:184:GLY:H	21:C:198:LYS:HZ1	1.65	0.45
21:C:342:MET:HE2	21:C:350:ILE:HD11	1.99	0.45
1:9:107:MET:HE1	24:9:610:CLA:HHC	1.99	0.45
1:AA:58:TYR:HB3	1:AA:78:TYR:HB3	1.99	0.45
4:v:216:HIS:CE1	24:v:609:CLA:C1A	3.00	0.45
24:v:601:CLA:HBA2	24:v:601:CLA:H3A	1.67	0.45
5:2:18:ILE:HG13	18:BA:110:PHE:CE2	2.52	0.45
24:A2:603:CLA:H203	24:A2:603:CLA:H162	1.80	0.45
28:A2:619:XAT:H203	24:BB:314:CLA:H72	1.99	0.45
24:BE:610:CLA:H92	24:BE:610:CLA:H61	1.76	0.45
23:BQ:607:CHL:HMA3	23:BQ:607:CHL:H43	1.99	0.45
24:BQ:611:CLA:CHA	24:BQ:611:CLA:HBA1	2.47	0.45
14:BV:76:LEU:HD11	14:BV:80:GLU:HB2	1.97	0.45
24:BV:603:CLA:HBA1	24:BV:603:CLA:H3A	1.80	0.45
23:Ba:309:CHL:HAB	26:Ba:318:NEX:H202	1.99	0.45
21:BF:362:ARG:HD2	21:BF:370:ARG:NH1	2.28	0.45
22:BU:256:PHE:CE2	22:BU:267:PRO:HG3	2.51	0.45
1:5:201:LEU:HD12	24:5:610:CLA:H11	1.98	0.44
1:5:227:PHE:O	1:5:231:VAL:HG12	2.17	0.44
2:6:142:LEU:HD12	2:6:143:ASP:N	2.32	0.44
23:6:606:CHL:HBD	23:6:606:CHL:HAA1	1.98	0.44
24:6:611:CLA:H2	24:6:612:CLA:HMD2	1.98	0.44
25:7:316:LUT:H161	25:7:316:LUT:H7	1.83	0.44
24:8:310:CLA:HBA2	24:8:310:CLA:CBD	2.42	0.44
23:G:607:CHL:H191	23:N:601:CHL:H41	1.98	0.44
14:S:262:PHE:HB3	30:C:501:LMG:H112	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:601:CHL:HBB1	23:S:601:CHL:CHC	2.45	0.44
15:T:8:PHE:CE1	29:b:601:BCR:H361	2.50	0.44
4:b:352:ARG:HH21	4:b:373:GLY:N	2.15	0.44
24:g:613:CLA:HMA1	25:g:615:LUT:H3	1.98	0.44
14:s:105:GLU:OE1	14:s:105:GLU:N	2.48	0.44
14:s:183:GLY:CA	24:s:608:CLA:HAB	2.47	0.44
23:s:605:CHL:HMC	23:s:606:CHL:NC	2.32	0.44
38:A:408:PHO:H141	38:A:408:PHO:H161	1.69	0.44
34:C:517:DGD:HB22	30:C:519:LMG:H291	1.99	0.44
22:r:140:GLU:OE2	22:r:247:ARG:NE	2.45	0.44
23:r:605:CHL:HBA1	26:r:617:NEX:H403	1.98	0.44
3:AB:194:TYR:HD1	3:AB:225:LYS:NZ	2.15	0.44
5:2:233:PHE:HE2	32:2:408:SQD:C45	2.30	0.44
8:Au:105:TRP:CD1	23:Au:609:CHL:HMD3	2.52	0.44
23:BB:310:CHL:C9	23:BB:310:CHL:H61	2.47	0.44
4:BE:352:ARG:HH21	4:BE:373:GLY:N	2.15	0.44
24:BE:605:CLA:HBA2	24:BE:605:CLA:H3A	1.28	0.44
24:BE:614:CLA:H61	24:BE:614:CLA:H41	1.48	0.44
8:BJ:57:LYS:HE3	8:BJ:63:SER:HB2	1.99	0.44
23:BQ:608:CHL:H51	23:BQ:608:CHL:H12	1.67	0.44
22:BU:284:ILE:O	22:BU:288:SER:N	2.45	0.44
2:6:108:PHE:HE2	24:6:604:CLA:CAC	2.16	0.44
2:6:172:GLY:C	1:7:62:PHE:HE1	2.26	0.44
2:6:172:GLY:C	1:7:62:PHE:CE1	2.95	0.44
24:7:304:CLA:H2	24:7:304:CLA:H62	1.70	0.44
24:S:602:CLA:CAB	25:S:615:LUT:H32	2.47	0.44
24:b:606:CLA:H62	24:b:606:CLA:H41	1.48	0.44
24:g:610:CLA:H3A	24:g:610:CLA:HBA2	1.33	0.44
24:n:610:CLA:H42	25:n:615:LUT:H26	1.98	0.44
14:s:241:ILE:HG21	24:s:612:CLA:HAC2	1.98	0.44
23:y:309:CHL:HAB	26:y:318:NEX:H202	1.98	0.44
21:C:269:GLU:OE2	21:C:444:HIS:ND1	2.44	0.44
29:C:514:BCR:H15C	29:C:514:BCR:H351	1.87	0.44
24:c:513:CLA:H91	24:c:513:CLA:H112	1.70	0.44
4:v:91:TRP:CE3	24:v:606:CLA:HBD	2.52	0.44
24:v:601:CLA:H141	24:v:601:CLA:H161	1.70	0.44
8:Au:216:LEU:HD23	8:Au:216:LEU:HA	1.82	0.44
23:Au:607:CHL:HBA1	23:Au:607:CHL:H3A	1.70	0.44
8:BB:238:LYS:HB3	8:BB:242:GLU:OE1	2.17	0.44
4:BE:18:ARG:HD3	4:BE:115:TRP:CH2	2.53	0.44
24:BJ:603:CLA:H92	24:BJ:603:CLA:H61	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BV:604:CLA:C1B	26:BV:616:NEX:H383	2.48	0.44
23:Ba:309:CHL:H143	23:Ba:309:CHL:H162	1.74	0.44
20:R:287:ALA:HA	20:R:290:ILE:HG22	1.99	0.44
21:1:130:ILE:HG23	21:1:134:LEU:HD23	1.99	0.44
21:1:216:SER:HB3	21:1:221:GLU:HG3	1.98	0.44
22:BU:67:TRP:CD1	22:BU:68:LEU:HG	2.50	0.44
3:8:106:GLY:O	3:8:110:MET:HG2	2.17	0.44
24:N:611:CLA:H93	24:N:611:CLA:H111	1.87	0.44
15:T:6:TYR:HA	15:T:9:LEU:HD12	2.00	0.44
4:b:164:PRO:HG3	24:b:607:CLA:O1D	2.18	0.44
32:d:406:SQD:H111	32:d:406:SQD:H142	1.55	0.44
24:g:612:CLA:HMC2	25:g:615:LUT:H11	1.99	0.44
24:n:602:CLA:HBA1	25:n:616:LUT:H382	2.00	0.44
21:C:396:MET:HG3	21:C:397:THR:N	2.32	0.44
24:C:508:CLA:H3A	24:C:508:CLA:HBA2	1.36	0.44
21:c:62:PHE:HB2	21:c:122:SER:OG	2.17	0.44
2:0:199:LEU:HD11	2:0:209:LEU:CD2	2.46	0.44
24:0:611:CLA:H2	24:0:612:CLA:HMD2	1.98	0.44
1:AA:61:PRO:HD2	23:AA:302:CHL:HBB2	1.99	0.44
3:AB:229:ILE:HD11	3:AB:233:ARG:NH2	2.32	0.44
4:v:90:LEU:HG	4:v:91:TRP:CD1	2.52	0.44
4:v:366:PHE:CD1	4:v:367:PRO:HD2	2.51	0.44
9:Av:56:ILE:HD13	9:Av:56:ILE:HA	1.87	0.44
5:BG:25:ARG:HD3	5:BG:26:ASP:N	2.31	0.44
8:BJ:173:GLU:HB3	23:BJ:609:CHL:HHB	1.98	0.44
24:BJ:610:CLA:H92	24:BJ:610:CLA:H61	1.75	0.44
25:BQ:615:LUT:H181	25:BQ:615:LUT:C8	2.47	0.44
28:BQ:619:XAT:H203	24:Ba:314:CLA:H72	1.99	0.44
14:BV:106:ASN:HB3	14:BV:110:TYR:HE1	1.82	0.44
24:BV:609:CLA:H3A	24:BV:609:CLA:CGA	2.47	0.44
8:Ba:59:LEU:HD23	8:Ba:59:LEU:HA	1.84	0.44
20:R:105:TRP:CE2	20:R:110:GLY:HA3	2.52	0.44
23:5:607:CHL:HBB1	23:6:601:CHL:H141	2.00	0.44
1:7:78:TYR:HB2	24:7:303:CLA:HMD3	2.00	0.44
1:7:80:TRP:CZ3	23:7:302:CHL:HBD	2.52	0.44
1:7:211:LEU:HB3	24:7:311:CLA:HMA2	2.00	0.44
4:B:164:PRO:HG3	24:B:606:CLA:O1D	2.16	0.44
8:G:238:LYS:HB3	8:G:242:GLU:CD	2.42	0.44
19:Z:5:PHE:O	19:Z:9:VAL:HG13	2.16	0.44
5:d:78:ALA:HB2	5:d:175:GLY:HA3	1.98	0.44
6:e:21:VAL:O	6:e:25:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:94:ARG:NH2	8:g:97:GLU:OE2	2.51	0.44
23:n:607:CHL:H3A	23:n:607:CHL:HBA1	1.54	0.44
14:s:72:PRO:HD3	23:s:601:CHL:HHC	1.98	0.44
14:s:76:LEU:HD11	14:s:80:GLU:HB2	1.99	0.44
14:s:229:GLY:O	14:s:233:MET:HG2	2.17	0.44
19:z:58:ASN:C	19:z:58:ASN:OD1	2.59	0.44
20:A:103:ASP:OD2	20:A:104:GLU:N	2.50	0.44
29:C:515:BCR:H15C	29:C:515:BCR:H351	1.83	0.44
22:r:170:LYS:O	22:r:174:VAL:HG22	2.18	0.44
22:r:207:ASN:HA	22:r:215:ARG:NH2	2.32	0.44
24:r:608:CLA:HBA2	24:r:608:CLA:H3A	1.48	0.44
1:9:236:THR:HB	1:9:238:LYS:NZ	2.32	0.44
2:0:70:GLU:OE1	2:0:70:GLU:N	2.48	0.44
24:AA:303:CLA:CGA	24:AA:303:CLA:H3A	2.47	0.44
29:v:617:BCR:H11C	29:v:617:BCR:H341	1.89	0.44
5:2:79:VAL:CG2	5:2:174:PHE:HB2	2.47	0.44
6:3:73:LEU:H	6:3:73:LEU:HD12	1.83	0.44
24:Au:602:CLA:HBA2	24:Au:602:CLA:H12	1.64	0.44
14:A6:66:ASP:N	14:A6:66:ASP:OD1	2.49	0.44
24:BB:313:CLA:HMC3	25:BB:316:LUT:H191	1.99	0.44
24:BE:603:CLA:H102	24:BE:610:CLA:H193	2.00	0.44
11:BN:58:VAL:O	11:BN:59:SER:OG	2.34	0.44
8:BQ:211:LEU:HD13	24:BQ:610:CLA:H3A	2.00	0.44
8:BQ:231:VAL:O	8:BQ:235:VAL:HG12	2.17	0.44
14:BV:106:ASN:HB3	14:BV:110:TYR:CE1	2.52	0.44
14:BV:201:HIS:CE1	14:BV:222:LYS:HD2	2.53	0.44
23:BV:605:CHL:OMC	25:BV:615:LUT:H163	2.18	0.44
24:Ba:314:CLA:HBA2	24:Ba:314:CLA:H3A	1.62	0.44
20:R:172:MET:HG3	20:R:182:PHE:CD2	2.53	0.44
29:R:410:BCR:H371	29:R:410:BCR:H24C	1.77	0.44
21:BF:162:GLY:HA3	21:BF:252:ILE:HG13	1.99	0.44
1:7:93:ALA:O	1:7:97:GLU:HG3	2.17	0.44
29:8:313:BCR:H11C	29:8:313:BCR:H341	1.88	0.44
8:G:119:LEU:HD23	8:G:119:LEU:HA	1.82	0.44
8:G:169:MET:CE	23:G:609:CHL:C1C	2.95	0.44
23:G:605:CHL:H3A	23:G:605:CHL:HBA2	1.44	0.44
32:L:103:SQD:H342	32:L:103:SQD:H312	1.51	0.44
24:S:602:CLA:HBA2	24:S:602:CLA:H3A	1.35	0.44
4:b:92:SER:OG	4:b:94:GLU:OE1	2.27	0.44
24:b:607:CLA:CGA	24:b:607:CLA:H3A	2.48	0.44
24:b:609:CLA:HBA2	24:b:609:CLA:H3A	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:27:VAL:HA	12:l:30:VAL:HG12	2.00	0.44
13:m:25:ILE:O	13:m:29:THR:HG23	2.18	0.44
24:n:610:CLA:HBA2	24:n:610:CLA:H12	1.48	0.44
21:c:221:GLU:N	21:c:221:GLU:OE1	2.51	0.44
22:r:216:LEU:HD12	22:r:216:LEU:O	2.16	0.44
4:v:371:VAL:HG12	4:v:377:VAL:HA	1.98	0.44
8:Au:247:HIS:CG	24:Au:613:CLA:HAA2	2.52	0.44
24:A2:610:CLA:H12	24:A2:610:CLA:HBA2	1.54	0.44
19:BC:50:LEU:HA	19:BC:53:LEU:HD12	1.98	0.44
24:BE:606:CLA:H62	24:BE:606:CLA:H41	1.47	0.44
24:BE:610:CLA:HBA2	24:BE:610:CLA:H3A	1.30	0.44
8:BJ:230:PHE:O	8:BJ:234:ILE:HG22	2.18	0.44
17:BY:125:GLU:OE1	17:BY:129:SER:HB2	2.17	0.44
24:Ba:305:CLA:H3A	24:Ba:305:CLA:HBA2	1.55	0.44
21:1:26:ARG:HD3	21:1:26:ARG:HA	1.57	0.44
21:1:369:LEU:HD13	21:1:380:LEU:HD23	1.99	0.44
21:BF:391:ARG:HD2	21:BF:395:TYR:CZ	2.52	0.44
24:5:611:CLA:H3A	24:5:611:CLA:HBA1	1.46	0.44
2:6:210:LYS:O	2:6:214:ILE:HG22	2.17	0.44
24:8:303:CLA:C4B	29:8:313:BCR:H281	2.47	0.44
4:B:28:ALA:HB2	4:B:107:CYS:HB2	1.99	0.44
24:B:603:CLA:H62	24:B:603:CLA:H41	1.76	0.44
14:S:188:TYR:HD1	23:S:607:CHL:CMC	2.30	0.44
14:S:188:TYR:O	23:S:607:CHL:HMC	2.18	0.44
8:Y:93:ALA:O	8:Y:97:GLU:HG3	2.18	0.44
8:g:226:MET:HE2	8:g:226:MET:HB3	1.44	0.44
23:n:607:CHL:H143	23:n:607:CHL:H111	1.71	0.44
21:c:457:LYS:HA	21:c:457:LYS:HD2	1.88	0.44
1:9:93:ALA:HA	1:9:96:ARG:CZ	2.48	0.44
24:0:611:CLA:C1B	27:0:617:LHG:HC31	2.47	0.44
4:v:60:MET:HE2	4:v:63:ILE:HD12	2.00	0.44
4:v:315:ILE:HG22	4:v:426:LEU:HB3	2.00	0.44
24:v:612:CLA:H162	24:v:612:CLA:H193	1.73	0.44
24:BE:602:CLA:H141	24:BE:602:CLA:H161	1.75	0.44
29:BE:620:BCR:H20C	29:BE:620:BCR:H361	1.82	0.44
21:1:327:ASN:OD1	21:1:330:SER:OG	2.23	0.44
20:BD:204:GLY:HA2	20:BD:278:TRP:HE1	1.83	0.44
24:BU:612:CLA:HMA1	25:BU:615:LUT:H22	1.98	0.44
3:8:196:GLY:O	3:8:200:PHE:HB2	2.18	0.44
27:G:618:LHG:H191	28:Y:301:XAT:H14	2.00	0.44
16:U:80:GLY:HA3	16:U:103:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:312:CLA:H61	24:Y:312:CLA:H41	1.88	0.44
4:b:208:LEU:HG	24:b:610:CLA:HMC1	1.99	0.44
24:b:613:CLA:H162	24:b:613:CLA:H193	1.82	0.44
24:b:613:CLA:HBA2	24:b:613:CLA:H3A	1.24	0.44
6:e:35:TRP:CD2	7:f:33:ALA:HB2	2.53	0.44
8:g:230:PHE:O	8:g:234:ILE:HG22	2.18	0.44
24:n:611:CLA:CHA	24:n:611:CLA:HBA1	2.47	0.44
24:C:513:CLA:H161	24:C:513:CLA:H141	1.66	0.44
2:0:99:HIS:HB3	2:0:221:MET:HE1	2.00	0.44
1:AA:74:PHE:HB3	1:AA:96:ARG:NH1	2.33	0.44
24:AA:305:CLA:H3A	24:AA:305:CLA:HBA2	1.39	0.44
4:v:224:ARG:CZ	4:v:224:ARG:HB2	2.47	0.44
24:v:604:CLA:H193	24:v:616:CLA:H201	2.00	0.44
24:v:607:CLA:H92	24:v:607:CLA:H62	1.66	0.44
29:v:619:BCR:H361	29:v:619:BCR:H20C	1.76	0.44
8:A2:165:GLN:HE22	23:A2:607:CHL:HMC	1.83	0.44
25:A6:615:LUT:H7	25:A6:615:LUT:H181	1.75	0.44
23:BJ:601:CHL:H41	27:BJ:618:LHG:H192	2.00	0.44
24:BQ:602:CLA:HBA1	25:BQ:616:LUT:H382	1.99	0.44
23:Ba:306:CHL:H3A	23:Ba:306:CHL:HBA2	1.56	0.44
24:BD:405:CLA:H72	24:BD:406:CLA:HBB1	1.99	0.44
22:BU:126:PRO:HG2	22:BU:127:TYR:HD1	1.82	0.44
1:5:231:VAL:HG11	24:5:613:CLA:CAC	2.47	0.44
3:8:223:ARG:NH1	3:8:224:LEU:HD23	2.32	0.44
4:B:91:TRP:CE3	24:B:606:CLA:HBD	2.52	0.44
4:B:120:LEU:HB2	4:B:123:PHE:CE2	2.52	0.44
4:B:191:ASP:HB3	4:B:194:VAL:HB	2.00	0.44
4:B:476:ARG:NH2	4:B:477:ASP:HA	2.33	0.44
5:D:18:ILE:HG13	18:X:110:PHE:CE2	2.52	0.44
5:D:108:LEU:CD2	6:E:76:LEU:HD11	2.47	0.44
5:D:257:ILE:HD13	5:D:257:ILE:HA	1.83	0.44
24:G:602:CLA:H111	24:G:602:CLA:H142	1.76	0.44
23:G:607:CHL:HBB2	23:G:609:CHL:CBC	2.44	0.44
23:N:607:CHL:H143	23:N:607:CHL:H111	1.76	0.44
24:S:602:CLA:CBB	25:S:615:LUT:H32	2.48	0.44
23:S:607:CHL:HHD	23:S:607:CHL:HBC2	2.00	0.44
8:Y:223:MET:HE2	24:Y:303:CLA:HMC2	1.99	0.44
4:b:121:GLU:CD	9:h:14:PRO:HB2	2.42	0.44
5:d:324:GLU:HG2	5:d:327:ARG:NH2	2.33	0.44
8:g:57:LYS:HE3	8:g:63:SER:HB2	1.99	0.44
11:k:34:ASN:O	11:k:37:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:231:VAL:O	8:n:235:VAL:HG12	2.17	0.44
25:n:615:LUT:H181	25:n:615:LUT:C8	2.47	0.44
24:C:511:CLA:HBD	24:C:511:CLA:CGA	2.47	0.44
27:C:520:LHG:H112	27:C:520:LHG:HC81	1.69	0.44
24:c:504:CLA:H172	24:c:511:CLA:HBB2	1.98	0.44
22:r:207:ASN:HA	22:r:215:ARG:HH22	1.83	0.44
2:0:132:ALA:O	2:0:135:GLN:HG2	2.18	0.44
24:v:608:CLA:H111	24:v:608:CLA:H91	1.65	0.44
24:v:614:CLA:H11	24:v:614:CLA:C1A	2.48	0.44
23:Au:606:CHL:HMC	25:Au:616:LUT:H163	1.99	0.44
8:BB:232:GLN:O	8:BB:236:THR:HG22	2.18	0.44
23:BB:309:CHL:H143	23:BB:309:CHL:H162	1.75	0.44
23:BB:310:CHL:H143	23:BB:310:CHL:H162	1.89	0.44
6:BH:37:PHE:CD1	6:BH:37:PHE:C	2.96	0.44
12:BO:13:LEU:N	13:BP:29:THR:HG21	2.33	0.44
21:1:68:ASN:HD22	21:1:68:ASN:C	2.26	0.44
21:1:157:MET:HE2	21:1:271:TYR:CE2	2.52	0.44
24:1:505:CLA:HBA2	24:1:505:CLA:H3A	1.58	0.44
24:5:610:CLA:H92	24:5:610:CLA:H61	1.77	0.44
1:7:75:PRO:HG3	1:7:212:LYS:HD3	2.00	0.44
1:7:107:MET:SD	25:7:316:LUT:C35	3.06	0.44
3:8:132:ALA:HB2	23:8:305:CHL:O2D	2.18	0.44
4:B:285:TYR:HE2	16:U:88:TYR:HA	1.83	0.44
27:L:102:LHG:H112	27:L:102:LHG:H142	1.66	0.44
24:b:605:CLA:HBB1	24:b:608:CLA:HAB	2.00	0.44
24:b:611:CLA:H102	24:b:616:CLA:HAA1	2.00	0.44
6:e:71:ASP:OD1	6:e:71:ASP:N	2.49	0.44
14:s:236:MET:HA	14:s:236:MET:HE2	2.00	0.44
8:y:175:TYR:CE1	8:y:182:PRO:HD3	2.53	0.44
20:a:260:PHE:CE1	20:a:263:ALA:HB2	2.53	0.44
21:c:36:TRP:O	24:c:509:CLA:H42	2.18	0.44
22:r:67:TRP:CD1	22:r:68:LEU:HG	2.50	0.44
1:9:214:LYS:HG2	24:9:611:CLA:OBD	2.18	0.44
23:9:607:CHL:HHC	23:9:607:CHL:HBB1	2.00	0.44
1:AA:93:ALA:O	1:AA:97:GLU:HG3	2.17	0.44
24:AA:305:CLA:C1C	26:AA:319:NEX:H222	2.48	0.44
3:AB:98:TYR:CD2	24:AB:301:CLA:HHB	2.53	0.44
3:AB:236:MET:HE3	24:AB:301:CLA:HMC2	2.00	0.44
24:v:601:CLA:H72	24:v:601:CLA:H111	1.75	0.44
24:v:606:CLA:H72	29:v:619:BCR:H321	2.00	0.44
24:v:615:CLA:H61	24:v:615:CLA:H41	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:v:617:BCR:H20C	29:v:617:BCR:H361	1.86	0.44
5:2:233:PHE:HD1	20:R:269:ARG:CZ	2.30	0.44
24:A6:608:CLA:H3A	24:A6:608:CLA:HBA2	1.48	0.44
4:BE:208:LEU:HG	24:BE:610:CLA:HMC1	2.00	0.44
4:BE:285:TYR:HE2	16:BX:88:TYR:HA	1.83	0.44
24:BE:605:CLA:HBB1	24:BE:608:CLA:HAB	1.99	0.44
8:BJ:226:MET:HE1	25:BJ:616:LUT:H10	2.00	0.44
14:BV:148:PHE:O	23:BV:606:CHL:HED1	2.18	0.44
24:Ba:314:CLA:H11	24:Ba:314:CLA:C4D	2.48	0.44
21:1:230:LEU:O	21:1:234:ILE:HG12	2.18	0.44
24:1:513:CLA:H122	29:1:514:BCR:H23C	2.00	0.44
1:5:93:ALA:HA	1:5:96:ARG:CZ	2.48	0.43
23:7:302:CHL:C3C	28:7:318:XAT:H222	2.47	0.43
3:8:120:GLN:CD	3:8:127:TRP:HD1	2.26	0.43
25:8:311:LUT:H11	25:8:311:LUT:H191	1.87	0.43
4:B:69:LEU:HD12	24:B:605:CLA:HBA1	2.00	0.43
4:B:74:SER:HA	4:B:92:SER:HB2	1.98	0.43
24:B:606:CLA:H111	24:B:606:CLA:H142	1.70	0.43
24:B:614:CLA:H11	24:B:614:CLA:C1A	2.48	0.43
8:G:173:GLU:HB3	23:G:609:CHL:HHB	1.99	0.43
8:N:187:GLU:CD	8:N:187:GLU:H	2.26	0.43
23:N:607:CHL:HBA1	23:N:607:CHL:H3A	1.45	0.43
23:g:608:CHL:HBA2	23:g:608:CHL:H3A	1.41	0.43
8:n:168:LEU:HD22	26:n:617:NEX:H15	2.00	0.43
24:y:314:CLA:H11	24:y:314:CLA:C4D	2.48	0.43
24:C:509:CLA:H93	24:C:509:CLA:H62	1.82	0.43
21:c:307:PRO:HB3	21:c:358:PHE:HB3	1.99	0.43
21:c:443:TRP:HE1	24:c:509:CLA:HED3	1.81	0.43
22:r:231:ASP:OD1	22:r:232:PRO:HD2	2.17	0.43
23:r:607:CHL:H3A	23:r:607:CHL:HBA2	1.55	0.43
1:9:105:TRP:CD1	23:9:609:CHL:HMD2	2.53	0.43
1:9:186:ALA:HB2	23:9:608:CHL:HBC1	1.99	0.43
24:9:604:CLA:HBA1	23:9:606:CHL:C1D	2.48	0.43
23:AA:309:CHL:HBA2	23:AA:309:CHL:H3A	1.48	0.43
24:2:402:CLA:H62	24:2:402:CLA:H41	1.57	0.43
8:Au:107:MET:HE3	25:Au:615:LUT:C34	2.48	0.43
14:A6:262:PHE:HB3	30:1:501:LMG:H112	1.99	0.43
4:BE:247:PHE:HE1	24:BE:603:CLA:H122	1.82	0.43
24:BJ:604:CLA:HBA1	24:BJ:604:CLA:H3A	1.80	0.43
8:BQ:97:GLU:OE2	23:BQ:609:CHL:HED1	2.17	0.43
14:BV:197:GLU:OE1	14:BV:197:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Ba:316:LUT:H35	25:Ba:316:LUT:H401	1.91	0.43
38:R:407:PHO:H141	38:R:407:PHO:H161	1.55	0.43
29:1:514:BCR:H20C	29:1:514:BCR:H361	1.82	0.43
20:BD:194:MET:HE3	20:BD:194:MET:HB3	1.93	0.43
21:BF:221:GLU:OE1	21:BF:221:GLU:N	2.50	0.43
29:BF:515:BCR:H24C	29:BF:515:BCR:H371	1.86	0.43
1:5:214:LYS:HG2	24:5:611:CLA:OBD	2.18	0.43
2:6:132:ALA:O	2:6:135:GLN:HG2	2.18	0.43
5:D:79:VAL:O	5:D:173:SER:OG	2.27	0.43
5:D:266:ARG:NH1	20:A:220:THR:HG23	2.16	0.43
6:E:73:LEU:H	6:E:73:LEU:HD12	1.83	0.43
28:N:619:XAT:C33	27:Y:319:LHG:H132	2.49	0.43
8:Y:155:ALA:HA	23:Y:306:CHL:C1C	2.48	0.43
8:Y:232:GLN:O	8:Y:236:THR:HG22	2.18	0.43
10:i:5:LYS:O	10:i:8:VAL:HG12	2.18	0.43
30:i:101:LMG:H341	30:i:101:LMG:H372	1.76	0.43
13:m:5:ILE:O	13:m:8:PHE:N	2.51	0.43
26:s:616:NEX:H181	26:s:616:NEX:C10	2.47	0.43
23:y:302:CHL:HBA1	23:y:302:CHL:H3A	1.62	0.43
24:y:304:CLA:HBA1	24:y:304:CLA:H3A	1.75	0.43
24:y:305:CLA:H3A	24:y:305:CLA:HBA2	1.48	0.43
20:A:328:MET:HE2	20:A:328:MET:HB3	1.67	0.43
22:r:273:THR:O	22:r:276:SER:OG	2.25	0.43
23:AA:302:CHL:C3C	28:AA:318:XAT:H222	2.47	0.43
3:AB:194:TYR:CD1	3:AB:225:LYS:NZ	2.86	0.43
4:v:150:CYS:SG	24:v:605:CLA:H202	2.58	0.43
8:Au:85:LEU:HB2	24:Au:602:CLA:H11	2.00	0.43
23:Au:601:CHL:HHC	23:Au:601:CHL:HBB1	1.99	0.43
8:BB:153:VAL:N	23:BB:306:CHL:O1D	2.35	0.43
4:BE:18:ARG:HD3	4:BE:115:TRP:CZ3	2.53	0.43
5:BG:90:LEU:H	5:BG:90:LEU:HD12	1.82	0.43
8:BJ:94:ARG:NH2	8:BJ:97:GLU:OE2	2.51	0.43
23:Ba:309:CHL:H193	23:Ba:309:CHL:H161	1.79	0.43
24:Ba:314:CLA:H2	24:Ba:314:CLA:H61	1.74	0.43
20:R:226:GLU:HB2	20:R:236:GLY:HA3	2.00	0.43
24:1:506:CLA:H12	29:1:515:BCR:H321	1.99	0.43
24:BD:405:CLA:H2A	24:BD:405:CLA:O1D	2.18	0.43
21:BF:82:TYR:OH	21:BF:394:GLU:OE2	2.36	0.43
1:5:162:TRP:O	1:5:166:VAL:HG13	2.19	0.43
2:6:167:MET:C	2:6:167:MET:SD	3.02	0.43
24:7:305:CLA:C1C	26:7:319:NEX:H222	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:312:CLA:HBA2	24:7:312:CLA:H3A	1.23	0.43
3:8:220:LYS:O	3:8:224:LEU:HG	2.18	0.43
4:B:256:MET:HA	4:B:256:MET:HE2	2.00	0.43
29:B:623:BCR:H20C	29:B:623:BCR:H361	1.83	0.43
24:G:610:CLA:HBA2	24:G:610:CLA:H3A	1.29	0.43
25:G:616:LUT:H181	25:G:616:LUT:H8	2.00	0.43
14:S:236:MET:HA	14:S:239:PHE:CD2	2.53	0.43
4:b:134:ASP:OD1	9:h:30:TYR:HA	2.18	0.43
24:b:610:CLA:H92	24:b:610:CLA:H61	1.77	0.43
29:b:619:BCR:H15C	29:b:619:BCR:H351	1.88	0.43
23:g:601:CHL:H41	27:g:618:LHG:H192	2.00	0.43
13:m:5:ILE:O	13:m:8:PHE:HB3	2.18	0.43
8:n:211:LEU:HD13	24:n:610:CLA:H3A	2.01	0.43
24:s:604:CLA:C1B	26:s:616:NEX:H383	2.48	0.43
24:y:303:CLA:H91	24:y:303:CLA:H111	1.81	0.43
21:c:134:LEU:HG	21:c:135:LEU:CD2	2.48	0.43
30:c:501:LMG:H212	24:c:504:CLA:C1B	2.48	0.43
24:r:614:CLA:HBA2	24:r:614:CLA:H3A	1.31	0.43
23:9:601:CHL:H3A	23:9:601:CHL:HBA1	1.44	0.43
2:0:91:LYS:NZ	1:AA:83:ALA:CA	2.81	0.43
2:0:209:LEU:HD11	24:0:610:CLA:HHB	2.00	0.43
1:AA:168:LEU:CD1	26:AA:319:NEX:H34	2.44	0.43
3:AB:228:GLU:OE2	24:AB:308:CLA:HMA1	2.17	0.43
25:AB:311:LUT:H35	25:AB:311:LUT:H401	1.83	0.43
5:2:133:LEU:O	5:2:137:VAL:HG22	2.18	0.43
27:Au:618:LHG:H191	28:BB:301:XAT:H14	2.00	0.43
17:A0:116:PHE:O	17:A0:120:THR:HG23	2.18	0.43
4:BE:226:TYR:HA	4:BE:231:MET:HG3	2.01	0.43
24:BE:609:CLA:H3A	24:BE:609:CLA:HBA2	1.61	0.43
24:BE:615:CLA:H91	24:BE:615:CLA:H112	1.73	0.43
5:BG:113:ALA:O	5:BG:117:LEU:HD22	2.18	0.43
5:BG:233:PHE:HB3	32:BG:406:SQD:H5	2.01	0.43
8:BJ:161:ILE:HD13	23:BJ:605:CHL:HAC1	2.00	0.43
24:BJ:612:CLA:HMC2	25:BJ:615:LUT:H11	2.00	0.43
14:BV:265:ASN:H	14:BV:268:THR:HG22	1.83	0.43
23:Ba:308:CHL:HBB2	23:Ba:310:CHL:CBC	2.49	0.43
34:1:517:DGD:HB22	30:1:519:LMG:H291	2.00	0.43
24:BF:514:CLA:H141	24:BF:514:CLA:H161	1.71	0.43
22:BU:76:TYR:CD2	24:BU:601:CLA:HAC1	2.52	0.43
27:6:617:LHG:H341	27:6:617:LHG:H372	1.58	0.43
1:7:61:PRO:HB3	14:BV:109:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:303:CLA:H3A	24:7:303:CLA:CGA	2.49	0.43
4:B:103:PHE:CE1	4:B:107:CYS:SG	3.11	0.43
29:B:617:BCR:H20C	29:B:617:BCR:H361	1.86	0.43
6:E:23:HIS:HA	6:E:26:THR:OG1	2.18	0.43
25:G:616:LUT:H11	25:G:616:LUT:H191	1.90	0.43
14:S:188:TYR:CE1	14:S:194:LEU:HG	2.39	0.43
8:Y:229:PHE:HE1	25:Y:316:LUT:H41	1.84	0.43
23:Y:310:CHL:C9	23:Y:310:CHL:C6	2.95	0.43
29:b:620:BCR:H20C	29:b:620:BCR:H361	1.81	0.43
5:d:80:SER:HA	5:d:173:SER:OG	2.18	0.43
14:s:122:MET:HE3	14:s:229:GLY:N	2.32	0.43
14:s:146:VAL:O	14:s:150:THR:HG23	2.18	0.43
14:s:197:GLU:OE1	14:s:197:GLU:N	2.51	0.43
8:y:111:LEU:HA	8:y:114:VAL:HG12	2.01	0.43
20:A:218:LEU:HD11	20:A:251:ALA:HB1	2.00	0.43
21:C:26:ARG:HD3	21:C:26:ARG:HA	1.47	0.43
20:a:82:ILE:HB	20:a:174:LEU:HB2	2.00	0.43
20:a:223:LEU:HD12	20:a:223:LEU:HA	1.84	0.43
21:c:26:ARG:HA	21:c:26:ARG:HD2	1.69	0.43
1:9:61:PRO:HD2	23:9:601:CHL:CBB	2.49	0.43
2:0:172:GLY:CA	1:AA:62:PHE:CZ	3.01	0.43
3:AB:120:GLN:CD	3:AB:127:TRP:HD1	2.26	0.43
4:v:467:ILE:HD13	4:v:467:ILE:HA	1.81	0.43
8:Au:186:ALA:HB2	23:Au:608:CHL:HBC1	1.99	0.43
28:Au:619:XAT:C34	27:A2:618:LHG:H132	2.48	0.43
29:Ay:102:BCR:H20C	29:Ay:102:BCR:H361	1.84	0.43
4:BE:164:PRO:HG3	24:BE:607:CLA:O1D	2.18	0.43
4:BE:188:GLU:OE1	4:BE:188:GLU:N	2.35	0.43
10:BL:7:PHE:O	10:BL:10:THR:OG1	2.30	0.43
14:BV:221:LEU:HB3	24:BV:609:CLA:CMA	2.48	0.43
15:BW:1:MET:SD	15:BW:2:GLU:N	2.92	0.43
20:BD:53:ILE:HD13	20:BD:53:ILE:HA	1.90	0.43
22:BU:253:PHE:CD2	28:BU:616:XAT:H12	2.53	0.43
24:BU:602:CLA:HBC1	27:BU:617:LHG:H281	1.99	0.43
1:5:128:GLU:HB3	1:5:137:GLN:NE2	2.32	0.43
1:5:223:MET:CE	24:5:602:CLA:HHC	2.44	0.43
23:5:609:CHL:HBC3	23:5:609:CHL:HMC	1.99	0.43
23:7:309:CHL:HMB3	26:7:319:NEX:H35	2.00	0.43
4:B:106:LEU:HD21	29:B:619:BCR:C13	2.49	0.43
24:B:608:CLA:H91	24:B:608:CLA:H111	1.65	0.43
23:G:606:CHL:HBB2	23:G:607:CHL:CBB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G:608:CHL:H62	23:G:608:CHL:H41	1.79	0.43
26:S:616:NEX:H181	26:S:616:NEX:H10	2.01	0.43
8:Y:153:VAL:N	23:Y:306:CHL:O1D	2.32	0.43
19:Z:6:GLN:O	19:Z:9:VAL:HG22	2.17	0.43
4:b:74:SER:HA	4:b:92:SER:HB2	2.00	0.43
4:b:156:PHE:HD2	24:b:607:CLA:HAC1	1.83	0.43
4:b:367:PRO:CB	5:d:346:VAL:CG1	2.97	0.43
5:d:133:LEU:HD23	5:d:133:LEU:HA	1.82	0.43
24:d:401:CLA:H72	24:a:407:CLA:HAB	2.00	0.43
14:s:123:LEU:CD2	24:s:604:CLA:HAB	2.49	0.43
14:s:148:PHE:O	23:s:606:CHL:HED1	2.18	0.43
25:s:615:LUT:H15	25:s:615:LUT:H201	1.91	0.43
20:a:131:TRP:CH2	24:c:506:CLA:HAA2	2.53	0.43
20:a:268:SER:O	20:a:272:HIS:ND1	2.41	0.43
21:c:391:ARG:HD2	21:c:395:TYR:CZ	2.53	0.43
24:r:601:CLA:HBC2	27:r:618:LHG:O7	2.19	0.43
1:9:126:PHE:CE1	1:9:147:LEU:HA	2.51	0.43
4:v:191:ASP:HB3	4:v:194:VAL:HB	2.00	0.43
4:v:296:GLN:N	4:v:296:GLN:CD	2.76	0.43
24:v:612:CLA:HBA2	24:v:612:CLA:H3A	1.24	0.43
14:A6:197:GLU:CD	14:A6:197:GLU:N	2.77	0.43
23:A6:607:CHL:HHD	23:A6:607:CHL:HBC2	1.99	0.43
26:BB:318:NEX:H15	26:BB:318:NEX:H201	1.89	0.43
8:BQ:90:GLU:O	8:BQ:94:ARG:HG2	2.18	0.43
14:BV:233:MET:HE3	24:BV:602:CLA:C2C	2.48	0.43
21:BF:307:PRO:HB3	21:BF:358:PHE:HB3	2.00	0.43
34:BF:518:DGD:HB31	30:BF:519:LMG:H321	2.00	0.43
24:5:604:CLA:H43	23:5:606:CHL:HBD	1.99	0.43
24:5:613:CLA:H11	24:5:613:CLA:CHA	2.48	0.43
2:6:162:PHE:HD1	23:6:606:CHL:O1D	2.01	0.43
2:6:238:PRO:O	2:6:241:ASN:HB2	2.19	0.43
23:6:601:CHL:H61	23:6:601:CHL:H41	1.60	0.43
3:8:223:ARG:CZ	3:8:224:LEU:HD23	2.49	0.43
24:B:601:CLA:H72	24:B:601:CLA:H111	1.74	0.43
24:N:602:CLA:H93	24:N:602:CLA:H111	1.71	0.43
24:N:611:CLA:H61	24:N:611:CLA:H41	1.77	0.43
8:Y:238:LYS:HB3	8:Y:242:GLU:OE1	2.18	0.43
24:Y:313:CLA:HMC3	25:Y:316:LUT:H191	2.00	0.43
4:b:18:ARG:HD3	4:b:115:TRP:CH2	2.54	0.43
24:b:612:CLA:H2A	24:b:612:CLA:HED2	1.99	0.43
9:h:22:LEU:HD22	9:h:23:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:105:TRP:CD1	23:n:609:CHL:HMD3	2.54	0.43
25:n:615:LUT:H35	25:n:615:LUT:H401	1.92	0.43
18:x:97:LEU:HD12	18:x:98:THR:N	2.32	0.43
32:A:413:SQD:H202	32:A:413:SQD:H172	1.64	0.43
24:C:512:CLA:H91	24:C:512:CLA:H112	1.71	0.43
29:a:411:BCR:H15C	29:a:411:BCR:H351	1.87	0.43
21:c:82:TYR:OH	21:c:394:GLU:OE2	2.36	0.43
2:0:90:ALA:HA	2:0:93:ARG:CZ	2.48	0.43
2:0:160:LEU:HD22	23:0:607:CHL:HBC1	2.00	0.43
25:0:616:LUT:H181	25:0:616:LUT:C8	2.48	0.43
4:v:264:PRO:HG2	4:v:267:LEU:HG	1.99	0.43
24:v:605:CLA:H193	24:v:609:CLA:HBB2	1.99	0.43
24:v:615:CLA:H72	29:v:619:BCR:H353	1.99	0.43
8:Au:171:ALA:O	8:Au:175:TYR:CD1	2.71	0.43
34:Av:102:DGD:HB62	34:Av:102:DGD:HB91	1.83	0.43
8:BB:155:ALA:HA	23:BB:306:CHL:C1C	2.48	0.43
4:BE:156:PHE:CD1	4:BE:156:PHE:N	2.87	0.43
4:BE:460:LEU:HD23	5:BG:285:LEU:HD12	2.00	0.43
24:BE:603:CLA:H62	24:BE:603:CLA:H41	1.86	0.43
6:BH:71:ASP:OD1	6:BH:71:ASP:N	2.50	0.43
8:BQ:227:PHE:O	8:BQ:231:VAL:HG12	2.18	0.43
14:BV:110:TYR:CD2	24:BV:602:CLA:H43	2.53	0.43
14:BV:174:ALA:O	14:BV:178:GLU:HG3	2.19	0.43
19:Bb:11:ALA:O	19:Bb:15:THR:HG22	2.18	0.43
24:BD:405:CLA:H72	24:BD:405:CLA:H111	1.78	0.43
21:BF:138:GLU:N	21:BF:138:GLU:OE1	2.52	0.43
21:BF:236:GLY:C	29:BF:516:BCR:H383	2.43	0.43
24:BF:505:CLA:HBA2	24:BF:505:CLA:H3A	1.59	0.43
2:6:187:LEU:H	2:6:187:LEU:HD22	1.84	0.43
24:6:610:CLA:H91	24:6:610:CLA:H111	1.79	0.43
1:7:58:TYR:HB3	1:7:78:TYR:HB3	2.00	0.43
1:7:236:THR:HG21	1:7:243:ASN:OD1	2.19	0.43
4:B:42:LEU:HD23	4:B:42:LEU:HA	1.68	0.43
24:B:608:CLA:HBA2	24:B:608:CLA:H3A	1.54	0.43
24:B:608:CLA:CMB	5:D:127:MET:HG2	2.49	0.43
24:B:613:CLA:H41	24:B:613:CLA:H61	1.53	0.43
29:B:623:BCR:HC42	32:a:412:SQD:H152	1.99	0.43
8:G:186:ALA:HB2	23:G:608:CHL:HBC1	2.00	0.43
9:H:47:MET:HE2	9:H:47:MET:N	2.34	0.43
13:M:1:MET:CE	13:M:3:VAL:H	2.32	0.43
8:N:191:TYR:CD2	24:N:610:CLA:O1D	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:155:ALA:C	4:b:156:PHE:HD1	2.27	0.43
24:b:610:CLA:H161	24:b:610:CLA:H141	1.72	0.43
6:e:56:PHE:HB2	20:a:312:ARG:HH22	1.83	0.43
8:g:106:ALA:CB	8:g:223:MET:HG2	2.45	0.43
24:g:602:CLA:HBA2	24:g:602:CLA:H12	1.70	0.43
12:l:13:LEU:N	13:m:29:THR:HG21	2.34	0.43
14:s:86:ASN:OD1	14:s:88:GLU:HG2	2.19	0.43
14:s:120:TRP:CE2	23:s:607:CHL:HED2	2.54	0.43
24:s:602:CLA:HBA2	24:s:602:CLA:H3A	1.19	0.43
21:C:391:ARG:HD2	21:C:395:TYR:CZ	2.54	0.43
24:a:405:CLA:H72	24:a:406:CLA:HBB1	2.01	0.43
4:v:69:LEU:HD12	24:v:605:CLA:HBA1	2.00	0.43
6:3:23:HIS:HA	6:3:26:THR:OG1	2.18	0.43
23:Au:601:CHL:H62	23:Au:601:CHL:H41	1.66	0.43
24:A2:614:CLA:HHC	24:A2:614:CLA:CBB	2.47	0.43
24:BE:615:CLA:H141	24:BE:615:CLA:H161	1.64	0.43
5:BG:68:TYR:O	7:BI:34:MET:HE2	2.18	0.43
19:Bb:18:ILE:HD12	19:Bb:18:ILE:HA	1.81	0.43
24:1:507:CLA:H161	24:1:507:CLA:H202	1.70	0.43
29:1:514:BCR:H24C	29:1:514:BCR:H371	1.86	0.43
20:BD:159:LEU:C	20:BD:162:PRO:HD2	2.43	0.43
24:BU:608:CLA:HBA2	24:BU:608:CLA:H3A	1.46	0.43
25:BU:615:LUT:H11	25:BU:615:LUT:H191	1.88	0.43
1:5:101:ILE:HG22	23:5:609:CHL:HMD2	1.99	0.43
1:5:188:ASP:OD1	1:5:191:TYR:N	2.42	0.43
2:6:234:THR:HB	2:6:257:PHE:HE2	1.83	0.43
3:8:235:ALA:O	3:8:238:ALA:HB3	2.18	0.43
8:G:110:ALA:CA	8:G:226:MET:HE1	2.49	0.43
14:S:239:PHE:HE1	25:S:614:LUT:H41	1.84	0.43
18:X:94:GLY:HA2	18:X:97:LEU:HD23	2.01	0.43
5:d:55:PHE:HB3	6:e:47:PHE:CD1	2.54	0.43
23:y:310:CHL:C9	23:y:310:CHL:H112	2.49	0.43
21:C:31:THR:HG21	21:C:41:ARG:HD3	2.00	0.43
24:C:508:CLA:H161	24:C:508:CLA:H141	1.69	0.43
29:a:411:BCR:H371	29:a:411:BCR:H24C	1.80	0.43
21:c:71:GLU:OE1	21:c:86:LEU:HA	2.19	0.43
24:c:508:CLA:H111	24:c:508:CLA:H142	1.84	0.43
29:c:515:BCR:H15C	29:c:515:BCR:H351	1.87	0.43
2:0:187:LEU:H	2:0:187:LEU:HD22	1.83	0.43
25:AA:317:LUT:H35	25:AA:317:LUT:H401	1.90	0.43
3:AB:152:LEU:O	3:AB:155:TRP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:90:LEU:HD23	4:v:91:TRP:H	1.84	0.43
4:v:201:HIS:HB2	24:v:602:CLA:C1B	2.49	0.43
23:Au:607:CHL:H121	23:A2:601:CHL:H201	2.00	0.43
34:Av:102:DGD:HB91	34:Av:102:DGD:HBW2	1.84	0.43
23:A2:601:CHL:H3A	23:A2:601:CHL:HBA1	1.42	0.43
25:BB:317:LUT:H11	25:BB:317:LUT:H191	1.93	0.43
4:BE:138:ILE:HA	4:BE:138:ILE:HD13	1.79	0.43
24:BE:603:CLA:H101	9:BK:58:LEU:HD12	2.00	0.43
27:BE:624:LHG:H142	27:BE:624:LHG:H112	1.80	0.43
5:BG:91:LEU:HD23	5:BG:110:GLY:HA2	2.01	0.43
23:BJ:601:CHL:H3A	23:BJ:601:CHL:HBA1	1.52	0.43
8:BQ:176:ARG:NH2	23:BQ:609:CHL:O1D	2.52	0.43
16:BX:80:GLY:HA3	16:BX:103:TYR:CD2	2.54	0.43
24:1:509:CLA:H142	24:1:509:CLA:H112	1.74	0.43
22:BU:170:LYS:HD3	22:BU:170:LYS:HA	1.79	0.43
22:BU:283:ILE:O	22:BU:286:THR:OG1	2.27	0.43
23:5:609:CHL:C3B	23:6:601:CHL:H2	2.49	0.43
24:5:613:CLA:C3B	25:5:615:LUT:H183	2.48	0.43
1:7:74:PHE:HB3	1:7:96:ARG:CZ	2.48	0.43
23:7:308:CHL:HBD	23:7:308:CHL:HAA1	2.00	0.43
4:B:315:ILE:HG22	4:B:426:LEU:HB3	1.99	0.43
8:G:171:ALA:O	8:G:175:TYR:CD1	2.72	0.43
28:G:619:XAT:C34	27:N:618:LHG:H132	2.49	0.43
23:Y:302:CHL:H3A	23:Y:302:CHL:HBA1	1.47	0.43
4:b:41:GLU:OE1	4:b:62:VAL:HG22	2.19	0.43
24:b:608:CLA:H92	24:b:608:CLA:H62	1.69	0.43
24:b:616:CLA:H2	24:b:616:CLA:H61	1.69	0.43
5:d:156:SER:HA	5:d:160:ILE:HG12	2.00	0.43
30:i:101:LMG:H391	24:c:507:CLA:H203	2.01	0.43
23:n:606:CHL:OMC	25:n:616:LUT:H163	2.19	0.43
20:A:164:GLY:HA3	20:A:294:ALA:HB1	2.00	0.43
21:C:184:GLY:H	21:C:198:LYS:NZ	2.17	0.43
21:c:67:MET:HE1	24:c:505:CLA:CHD	2.49	0.43
24:c:502:CLA:HBA2	24:c:502:CLA:H3A	1.18	0.43
1:9:105:TRP:CD1	23:9:608:CHL:HED3	2.54	0.43
24:9:613:CLA:C3B	25:9:615:LUT:H183	2.49	0.43
23:0:608:CHL:H3A	23:0:608:CHL:HBA2	1.77	0.43
27:0:617:LHG:H372	27:0:617:LHG:H341	1.57	0.43
3:AB:157:GLU:HG2	3:AB:160:ARG:HH12	1.84	0.43
24:AB:308:CLA:HBB2	25:AB:311:LUT:H34	2.00	0.43
24:v:609:CLA:H3A	24:v:609:CLA:HBA2	1.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Au:110:ALA:HB1	25:Au:615:LUT:H12	2.01	0.43
25:Au:616:LUT:H181	25:Au:616:LUT:H8	2.00	0.43
29:Ay:102:BCR:H15C	29:Ay:102:BCR:H351	1.83	0.43
4:BE:285:TYR:CE2	16:BX:88:TYR:HA	2.54	0.43
24:BE:607:CLA:H3A	24:BE:607:CLA:CGA	2.48	0.43
24:BE:611:CLA:H13	24:BE:613:CLA:H12	2.00	0.43
8:BJ:227:PHE:O	8:BJ:231:VAL:HG12	2.18	0.43
29:BK:101:BCR:H20C	29:BK:101:BCR:H361	1.82	0.43
29:BK:101:BCR:H24C	29:BK:101:BCR:H371	1.79	0.43
10:BL:29:GLY:O	10:BL:34:ARG:NE	2.52	0.43
24:BQ:602:CLA:H161	24:BQ:602:CLA:H141	1.87	0.43
24:BV:608:CLA:H3A	24:BV:608:CLA:HBA2	1.61	0.43
23:Ba:306:CHL:HAA1	23:Ba:306:CHL:HBD	2.01	0.43
20:R:103:ASP:OD2	20:R:104:GLU:N	2.52	0.43
21:1:391:ARG:HD2	21:1:395:TYR:CZ	2.53	0.43
24:1:506:CLA:H61	24:1:506:CLA:H92	1.75	0.43
24:1:508:CLA:HBA2	24:1:508:CLA:H3A	1.37	0.43
24:BF:506:CLA:H61	24:BF:506:CLA:H92	1.69	0.43
2:6:167:MET:SD	2:6:171:GLU:HG3	2.59	0.43
1:7:204:ASP:HB3	1:7:207:ALA:HB3	2.01	0.43
24:7:304:CLA:OBD	23:7:310:CHL:HBA2	2.19	0.43
25:7:317:LUT:H15	25:7:317:LUT:H201	1.89	0.43
3:8:239:MET:HE3	3:8:239:MET:O	2.19	0.43
25:8:311:LUT:H31	25:8:311:LUT:H391	1.92	0.43
4:B:18:ARG:NH1	12:L:5:ASN:HD22	2.17	0.43
8:N:58:TYR:CZ	8:N:59:LEU:CD2	3.02	0.43
8:n:207:ALA:O	8:n:211:LEU:HG	2.19	0.43
8:y:119:LEU:HD13	8:y:119:LEU:HA	1.92	0.43
29:A:411:BCR:H11C	29:A:411:BCR:H341	1.92	0.43
21:C:68:ASN:C	21:C:68:ASN:HD22	2.27	0.43
2:0:172:GLY:O	2:0:175:ILE:N	2.51	0.43
2:0:209:LEU:HG	24:0:610:CLA:HMA2	2.00	0.43
2:0:210:LYS:O	2:0:214:ILE:HG22	2.18	0.43
1:AA:78:TYR:HB2	24:AA:303:CLA:HMD3	2.00	0.43
4:v:237:VAL:HG23	24:v:612:CLA:HMD3	2.01	0.43
24:2:403:CLA:H112	24:2:403:CLA:H91	1.71	0.43
7:4:22:VAL:HB	7:4:23:PRO:HD3	2.01	0.43
28:A2:619:XAT:C33	27:BB:319:LHG:H132	2.49	0.43
16:A8:88:TYR:HB3	16:A8:100:ILE:HD12	2.01	0.43
24:BB:304:CLA:H3A	24:BB:304:CLA:HBA1	1.80	0.43
4:BE:127:ARG:NH2	9:BK:30:TYR:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BL:101:LMG:H391	24:BF:507:CLA:H203	2.01	0.43
24:BQ:611:CLA:H62	24:BQ:612:CLA:C1D	2.49	0.43
14:BV:206:PHE:O	25:BV:614:LUT:H24	2.19	0.43
17:BY:110:GLY:HA3	27:BY:201:LHG:H181	2.00	0.43
24:BF:507:CLA:H61	24:BF:507:CLA:H92	1.80	0.43
24:5:604:CLA:HBA1	23:5:606:CHL:C1D	2.49	0.42
23:5:607:CHL:HBA1	23:5:607:CHL:H3A	1.36	0.42
2:6:73:GLY:C	24:6:602:CLA:HED3	2.44	0.42
23:6:607:CHL:H3A	23:6:607:CHL:HBA1	1.40	0.42
24:6:611:CLA:C1B	27:6:617:LHG:HC31	2.49	0.42
3:8:110:MET:CE	3:8:231:HIS:HB3	2.47	0.42
23:8:306:CHL:HBA2	23:8:306:CHL:H3A	1.39	0.42
4:B:90:LEU:HD23	4:B:91:TRP:H	1.84	0.42
24:B:611:CLA:H2A	24:B:611:CLA:O2D	2.19	0.42
5:D:343:PRO:O	5:D:346:VAL:HG22	2.19	0.42
6:E:56:PHE:HB2	20:A:312:ARG:NH2	2.33	0.42
34:H:102:DGD:HBT2	34:H:102:DGD:HB72	1.76	0.42
23:N:606:CHL:HBA1	23:N:606:CHL:H3A	1.86	0.42
14:S:92:ASP:OD2	14:S:92:ASP:C	2.62	0.42
16:U:88:TYR:HB3	16:U:100:ILE:HD12	2.01	0.42
18:X:94:GLY:O	18:X:97:LEU:HG	2.19	0.42
8:Y:250:ASP:OD1	8:Y:253:ASN:OD1	2.36	0.42
24:Y:314:CLA:HBA2	24:Y:314:CLA:H3A	1.72	0.42
7:f:22:VAL:HB	7:f:23:PRO:HD3	2.00	0.42
8:g:161:ILE:HD13	23:g:605:CHL:HAC1	2.01	0.42
23:g:601:CHL:H202	23:g:601:CHL:H161	1.69	0.42
8:n:241:ILE:H	8:n:241:ILE:HG13	1.63	0.42
8:y:104:ARG:HB3	23:y:309:CHL:HED1	2.01	0.42
28:y:301:XAT:H15	28:y:301:XAT:H201	1.85	0.42
20:A:183:MET:HB3	24:A:405:CLA:HBC2	2.01	0.42
20:A:226:GLU:HB2	20:A:236:GLY:HA3	2.00	0.42
38:A:408:PHO:H61	38:A:408:PHO:H2	1.61	0.42
24:a:406:CLA:HED2	24:a:406:CLA:H2A	2.00	0.42
21:c:67:MET:HE1	24:c:505:CLA:C1D	2.49	0.42
1:AA:223:MET:HE2	1:AA:223:MET:HB2	1.85	0.42
23:AA:307:CHL:HBB1	25:AA:317:LUT:H161	2.00	0.42
23:Au:601:CHL:C10	23:Au:601:CHL:H61	2.49	0.42
8:A2:229:PHE:HE1	25:A2:615:LUT:H41	1.84	0.42
14:A6:158:ASN:OD1	14:A6:158:ASN:N	2.50	0.42
14:A6:202:PRO:HG3	23:A6:607:CHL:HHD	2.01	0.42
4:BE:223:GLN:HB2	4:BE:224:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:21:VAL:O	6:BH:25:ILE:HG12	2.18	0.42
6:BH:56:PHE:HB2	20:BD:312:ARG:HH22	1.82	0.42
23:BJ:601:CHL:HHC	23:BJ:601:CHL:HBB1	2.00	0.42
13:BP:5:ILE:O	13:BP:8:PHE:HB3	2.19	0.42
24:1:508:CLA:H43	24:1:511:CLA:HAC1	2.01	0.42
20:BD:260:PHE:CE1	20:BD:263:ALA:HB2	2.54	0.42
21:BF:63:TRP:CZ2	21:BF:67:MET:HG3	2.54	0.42
22:BU:132:GLY:O	22:BU:135:ARG:HB2	2.19	0.42
23:6:606:CHL:H3A	23:6:606:CHL:HBA2	1.55	0.42
23:7:307:CHL:HBB1	25:7:317:LUT:H161	2.00	0.42
24:B:608:CLA:H141	24:B:608:CLA:H161	1.90	0.42
10:I:7:PHE:O	10:I:11:VAL:HG22	2.19	0.42
29:K:101:BCR:H15C	29:K:101:BCR:H351	1.89	0.42
29:K:102:BCR:H24C	29:K:102:BCR:H371	1.87	0.42
13:M:8:PHE:HD2	13:M:8:PHE:C	2.27	0.42
14:S:132:GLU:CD	14:S:251:VAL:HB	2.45	0.42
26:S:616:NEX:H181	26:S:616:NEX:C10	2.49	0.42
4:b:368:VAL:HG21	4:b:422:ARG:HG2	2.00	0.42
24:b:602:CLA:H111	24:b:602:CLA:H72	1.74	0.42
23:n:609:CHL:H193	23:n:609:CHL:H162	1.72	0.42
8:y:168:LEU:O	8:y:172:VAL:HG13	2.19	0.42
23:y:302:CHL:H202	23:y:302:CHL:H161	1.67	0.42
21:C:230:LEU:O	21:C:234:ILE:HG12	2.19	0.42
22:r:195:GLU:O	22:r:199:ILE:HD12	2.18	0.42
24:r:603:CLA:H91	24:r:603:CLA:H112	1.83	0.42
2:0:120:VAL:C	2:0:121:ARG:HE	2.27	0.42
3:AB:127:TRP:HE1	3:AB:252:PRO:HD3	1.84	0.42
29:4:101:BCR:H361	29:4:101:BCR:H20C	1.78	0.42
9:Av:40:THR:O	9:Av:43:MET:HB2	2.19	0.42
14:A6:236:MET:HA	14:A6:239:PHE:CD2	2.54	0.42
24:A6:604:CLA:C1C	26:A6:616:NEX:H222	2.49	0.42
24:BB:313:CLA:H61	24:BB:313:CLA:H102	1.76	0.42
5:BG:140:ARG:HD2	20:BD:225:ARG:NH1	2.34	0.42
32:BG:406:SQD:H142	32:BG:406:SQD:H111	1.53	0.42
27:BQ:618:LHG:H341	27:BQ:618:LHG:H312	1.95	0.42
24:Ba:304:CLA:H3A	24:Ba:304:CLA:HBA1	1.76	0.42
24:BD:406:CLA:HED2	24:BD:406:CLA:H2A	2.01	0.42
23:BU:607:CHL:HBA2	23:BU:607:CHL:H3A	1.55	0.42
27:BU:617:LHG:H161	27:BU:617:LHG:H132	1.71	0.42
24:5:602:CLA:HMC3	24:5:602:CLA:HBC3	2.00	0.42
2:6:75:TYR:HE2	23:6:601:CHL:HBC2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:177:GLY:HA2	23:6:608:CHL:HMC	2.00	0.42
2:6:219:LEU:HD22	24:6:611:CLA:HHD	2.01	0.42
1:7:175:TYR:HB3	23:7:309:CHL:CMC	2.49	0.42
24:8:303:CLA:NB	29:8:313:BCR:H281	2.34	0.42
23:8:307:CHL:HHC	23:8:307:CHL:HBB1	2.00	0.42
13:M:15:ILE:HD12	13:M:15:ILE:O	2.19	0.42
8:N:202:ALA:HB2	24:N:610:CLA:HAA2	2.00	0.42
8:N:229:PHE:HE1	25:N:615:LUT:H41	1.84	0.42
27:N:618:LHG:H341	27:N:618:LHG:H312	1.86	0.42
19:Z:50:LEU:HD23	19:Z:53:LEU:HD12	2.00	0.42
24:b:602:CLA:H142	24:b:602:CLA:H112	1.65	0.42
9:h:24:LYS:HA	9:h:24:LYS:HD3	1.76	0.42
8:y:214:LYS:HD2	24:y:313:CLA:HBD	2.01	0.42
24:y:314:CLA:H61	24:y:314:CLA:H2	1.74	0.42
29:A:411:BCR:H20C	29:A:411:BCR:H361	1.84	0.42
24:C:513:CLA:H122	29:C:514:BCR:H23C	2.00	0.42
21:c:148:GLY:O	21:c:156:LYS:NZ	2.49	0.42
24:c:509:CLA:HBC3	24:c:511:CLA:H92	2.02	0.42
1:9:107:MET:HG3	1:9:222:ALA:HB2	2.01	0.42
24:9:613:CLA:H11	24:9:613:CLA:CHA	2.49	0.42
2:0:142:LEU:HD12	2:0:143:ASP:N	2.33	0.42
25:AB:311:LUT:H15	25:AB:311:LUT:H201	1.87	0.42
24:v:611:CLA:O2D	24:v:611:CLA:H2A	2.19	0.42
24:v:614:CLA:H192	24:v:614:CLA:H162	1.91	0.42
29:v:617:BCR:H15C	29:v:617:BCR:H351	1.79	0.42
5:2:181:ARG:HH21	5:2:334:ASP:CG	2.27	0.42
8:Au:214:LYS:O	8:Au:218:ASN:ND2	2.50	0.42
24:Au:602:CLA:H141	24:Au:602:CLA:H161	1.69	0.42
8:A2:58:TYR:CZ	8:A2:59:LEU:CD2	3.03	0.42
8:A2:165:GLN:NE2	23:A2:607:CHL:HMC	2.35	0.42
24:A2:603:CLA:H92	24:A2:603:CLA:H61	1.82	0.42
8:BB:94:ARG:HD2	8:BB:94:ARG:N	2.34	0.42
8:BB:134:ALA:O	8:BB:137:GLN:HG3	2.20	0.42
8:BB:223:MET:HE1	24:BB:303:CLA:HHC	2.02	0.42
26:BB:320:NEX:H28	23:BU:605:CHL:HBA2	2.00	0.42
4:BE:198:ILE:H	4:BE:198:ILE:HD12	1.84	0.42
5:BG:80:SER:HA	5:BG:173:SER:OG	2.18	0.42
5:BG:233:PHE:N	20:BD:269:ARG:HH11	2.18	0.42
5:BG:234:ARG:HH11	32:BG:406:SQD:H61	1.85	0.42
24:BG:401:CLA:H72	24:BD:407:CLA:HAB	2.01	0.42
24:BJ:602:CLA:H3A	24:BJ:602:CLA:HBA2	1.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BL:101:LMG:H341	30:BL:101:LMG:H372	1.75	0.42
23:BQ:605:CHL:HBD	23:BQ:605:CHL:HAA1	2.02	0.42
23:BQ:607:CHL:H111	23:BQ:607:CHL:H143	1.71	0.42
14:BV:183:GLY:CA	24:BV:608:CLA:HAB	2.48	0.42
8:Ba:191:TYR:HB3	24:Ba:311:CLA:HED2	2.01	0.42
21:1:119:LEU:HD12	21:1:119:LEU:HA	1.86	0.42
21:1:311:GLN:NE2	21:1:358:PHE:O	2.52	0.42
21:BF:134:LEU:HG	21:BF:135:LEU:CD2	2.49	0.42
21:BF:156:LYS:HD2	21:BF:156:LYS:HA	1.87	0.42
23:5:607:CHL:HBB1	23:5:607:CHL:HHC	2.02	0.42
1:7:230:PHE:O	1:7:234:ILE:HG22	2.19	0.42
4:B:157:HIS:HA	4:B:163:GLY:HA3	2.01	0.42
4:B:224:ARG:CZ	4:B:224:ARG:HB2	2.46	0.42
24:B:615:CLA:H93	24:B:615:CLA:H111	1.72	0.42
8:G:91:THR:HG22	8:G:95:ASN:ND2	2.34	0.42
23:G:601:CHL:H161	23:G:601:CHL:H202	1.75	0.42
24:G:613:CLA:H61	24:G:613:CLA:H2	1.70	0.42
23:N:607:CHL:H121	23:Y:302:CHL:H18	2.00	0.42
24:S:604:CLA:CHA	24:S:604:CLA:HBA1	2.49	0.42
15:T:11:VAL:HG12	29:b:601:BCR:H363	2.00	0.42
8:Y:105:TRP:HD1	23:Y:310:CHL:HMD2	1.84	0.42
23:Y:306:CHL:HBA2	23:Y:306:CHL:H3A	1.47	0.42
9:h:20:GLY:O	9:h:24:LYS:HG2	2.19	0.42
14:s:106:ASN:O	14:s:110:TYR:CD1	2.73	0.42
14:s:233:MET:HE3	24:s:602:CLA:C2C	2.49	0.42
20:a:188:ALA:HB2	20:a:328:MET:HB2	2.01	0.42
21:c:240:LEU:HD11	24:c:502:CLA:CAB	2.49	0.42
24:c:507:CLA:H143	24:c:507:CLA:H162	1.75	0.42
24:r:610:CLA:HBA2	24:r:610:CLA:H3A	1.25	0.42
27:r:618:LHG:H161	27:r:618:LHG:H132	1.74	0.42
1:9:134:ALA:O	1:9:137:GLN:HG2	2.20	0.42
24:0:610:CLA:HMB3	24:0:612:CLA:HAA1	2.01	0.42
3:AB:235:ALA:O	3:AB:238:ALA:HB3	2.19	0.42
29:v:622:BCR:HC42	32:BD:412:SQD:H152	1.99	0.42
6:3:67:THR:HG22	6:3:75:GLN:HE22	1.84	0.42
24:Au:602:CLA:HBA2	24:Au:602:CLA:H3A	1.40	0.42
16:A8:102:ARG:HG2	16:A8:103:TYR:H	1.84	0.42
8:BJ:227:PHE:HE2	24:BJ:602:CLA:H18	1.85	0.42
24:BQ:610:CLA:H62	24:BQ:612:CLA:CBA	2.44	0.42
8:Ba:208:PHE:HA	8:Ba:211:LEU:HD12	2.00	0.42
23:Ba:308:CHL:HBA1	23:Ba:308:CHL:H3A	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Bb:46:LEU:O	19:Bb:50:LEU:HD13	2.19	0.42
38:BD:409:PHO:H71	38:BD:409:PHO:H112	1.74	0.42
21:BF:36:TRP:O	24:BF:509:CLA:H42	2.19	0.42
24:BU:603:CLA:H93	24:BU:603:CLA:H61	1.87	0.42
2:6:62:GLN:OE1	2:6:62:GLN:N	2.52	0.42
25:6:616:LUT:H181	25:6:616:LUT:C8	2.49	0.42
24:7:303:CLA:CBB	25:7:317:LUT:H32	2.49	0.42
24:7:305:CLA:C1B	26:7:319:NEX:H383	2.50	0.42
25:7:317:LUT:H11	25:7:317:LUT:H191	1.94	0.42
3:8:145:LEU:HD12	3:8:145:LEU:O	2.19	0.42
29:8:313:BCR:H15C	29:8:313:BCR:H351	1.93	0.42
9:H:24:LYS:HD3	9:H:24:LYS:HA	1.74	0.42
17:W:116:PHE:O	17:W:120:THR:HG23	2.19	0.42
4:b:18:ARG:HD3	4:b:115:TRP:CZ3	2.54	0.42
24:b:605:CLA:H92	24:b:605:CLA:H61	1.87	0.42
5:d:140:ARG:HD2	20:a:225:ARG:NH2	2.34	0.42
24:C:506:CLA:H43	29:C:515:BCR:H323	2.02	0.42
24:C:506:CLA:H61	24:C:506:CLA:H92	1.74	0.42
24:C:506:CLA:H12	29:C:515:BCR:H321	2.00	0.42
24:C:507:CLA:HMA2	24:C:507:CLA:H2	2.01	0.42
2:0:167:MET:SD	2:0:167:MET:C	3.02	0.42
24:0:613:CLA:H8	24:0:613:CLA:H51	1.81	0.42
1:AA:175:TYR:HB3	23:AA:309:CHL:CMC	2.49	0.42
1:AA:236:THR:HG21	1:AA:243:ASN:OD1	2.18	0.42
23:AA:308:CHL:HAA1	23:AA:308:CHL:HBD	2.00	0.42
3:AB:132:ALA:HB2	23:AB:305:CHL:O2D	2.18	0.42
5:2:78:ALA:HB2	5:2:175:GLY:HA3	2.01	0.42
24:A6:602:CLA:CAB	25:A6:615:LUT:H32	2.49	0.42
18:BA:94:GLY:O	18:BA:97:LEU:HG	2.19	0.42
4:BE:74:SER:HA	4:BE:92:SER:HB2	2.01	0.42
4:BE:368:VAL:HG21	4:BE:422:ARG:HG2	2.02	0.42
5:BG:349:ARG:HD3	5:BG:353:LEU:HD11	2.00	0.42
7:BI:11:THR:HG23	7:BI:14:TRP:H	1.85	0.42
24:BJ:613:CLA:HMA1	25:BJ:615:LUT:H3	2.00	0.42
9:BK:32:LYS:HD2	9:BK:32:LYS:HA	1.63	0.42
13:BP:5:ILE:O	13:BP:8:PHE:N	2.53	0.42
23:Ba:308:CHL:H143	23:Ba:308:CHL:H111	1.78	0.42
38:R:407:PHO:H2	38:R:407:PHO:H61	1.62	0.42
30:1:501:LMG:H212	24:1:504:CLA:C2B	2.49	0.42
20:BD:186:PHE:HE1	20:BD:192:ILE:HD13	1.84	0.42
20:BD:202:VAL:HA	20:BD:205:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BF:209:ILE:HD12	21:BF:209:ILE:HA	1.85	0.42
24:BF:509:CLA:H43	24:BF:512:CLA:HAC1	2.02	0.42
24:BU:601:CLA:HBC2	27:BU:617:LHG:O7	2.19	0.42
24:BU:610:CLA:H3A	24:BU:610:CLA:HBA2	1.24	0.42
1:5:107:MET:HE1	24:5:610:CLA:HAB	2.01	0.42
1:5:176:ARG:NH1	23:5:609:CHL:HED1	2.33	0.42
2:6:83:SER:HB3	2:6:89:PHE:CD1	2.54	0.42
24:7:311:CLA:H3A	24:7:311:CLA:CGA	2.50	0.42
24:B:603:CLA:C3D	24:B:605:CLA:H43	2.49	0.42
24:B:609:CLA:HBA2	24:B:609:CLA:H3A	1.29	0.42
24:B:614:CLA:H62	24:B:614:CLA:H41	1.62	0.42
5:D:90:LEU:HG	9:H:62:ASN:ND2	2.34	0.42
29:K:102:BCR:H373	21:C:55:ALA:HB1	2.01	0.42
25:N:615:LUT:H35	25:N:615:LUT:H401	1.90	0.42
4:b:234:ILE:O	4:b:237:VAL:HG22	2.20	0.42
24:b:607:CLA:H142	24:b:607:CLA:H111	1.68	0.42
5:d:140:ARG:HD2	20:a:225:ARG:NH1	2.35	0.42
10:i:1:MET:HA	10:i:1:MET:HE2	2.02	0.42
14:s:144:GLU:OE2	14:s:149:LYS:HD3	2.19	0.42
38:A:408:PHO:H92	38:A:408:PHO:H62	1.85	0.42
21:C:300:GLU:OE1	21:C:300:GLU:N	2.45	0.42
21:c:342:MET:HE1	21:c:356:MET:HE3	2.02	0.42
22:r:207:ASN:HD22	24:r:614:CLA:HBC3	1.84	0.42
1:AA:107:MET:SD	25:AA:316:LUT:C35	3.07	0.42
23:AA:302:CHL:HBB1	23:AA:302:CHL:CHC	2.47	0.42
23:AA:302:CHL:H3A	23:AA:302:CHL:HBA1	1.62	0.42
3:AB:83:PHE:HE2	28:AB:312:XAT:H383	1.84	0.42
24:v:616:CLA:H51	24:v:616:CLA:H11	1.86	0.42
8:Au:119:LEU:HD23	8:Au:119:LEU:HA	1.82	0.42
24:Au:613:CLA:H2	24:Au:613:CLA:H61	1.69	0.42
18:BA:94:GLY:HA2	18:BA:97:LEU:HD23	2.01	0.42
8:BB:108:LEU:HD23	8:BB:108:LEU:HA	1.82	0.42
19:BC:6:GLN:O	19:BC:9:VAL:HG22	2.20	0.42
19:BC:19:LEU:O	19:BC:23:VAL:HG23	2.20	0.42
4:BE:367:PRO:CB	5:BG:346:VAL:CG1	2.98	0.42
24:BE:613:CLA:H3A	24:BE:613:CLA:HBA2	1.24	0.42
6:BH:69:ARG:CB	16:BX:102:ARG:HH12	2.31	0.42
7:BI:22:VAL:HB	7:BI:23:PRO:HD3	2.02	0.42
14:BV:188:TYR:HB3	23:BV:607:CHL:HHC	2.01	0.42
14:BV:224:LYS:HE2	24:BV:611:CLA:HBD	2.01	0.42
8:Ba:169:MET:CE	23:Ba:310:CHL:C1C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ba:308:CHL:H203	23:Ba:308:CHL:H161	1.69	0.42
21:1:447:ARG:HD3	24:1:508:CLA:HED2	2.01	0.42
20:BD:131:TRP:CH2	24:BF:506:CLA:HAA2	2.55	0.42
22:BU:209:GLU:CD	22:BU:214:LYS:HB3	2.45	0.42
2:6:171:GLU:HB3	23:6:609:CHL:HHB	2.02	0.42
23:6:608:CHL:H3A	23:6:608:CHL:HBA2	1.79	0.42
4:B:103:PHE:HZ	24:B:615:CLA:H2	1.84	0.42
24:B:609:CLA:H62	24:B:609:CLA:H41	1.75	0.42
29:B:617:BCR:H342	29:B:623:BCR:H402	2.01	0.42
8:Y:188:ASP:OD1	8:Y:190:LEU:N	2.49	0.42
19:Z:31:ASP:OD1	19:Z:34:SER:HB3	2.19	0.42
4:b:216:HIS:HE1	24:b:610:CLA:C1A	2.32	0.42
24:b:615:CLA:H91	24:b:615:CLA:H112	1.74	0.42
5:d:230:ALA:HA	21:c:457:LYS:HZ3	1.78	0.42
5:d:233:PHE:HE1	20:a:270:SER:HA	1.84	0.42
8:g:165:GLN:HG3	23:g:606:CHL:HMA3	2.01	0.42
10:i:14:PHE:CE2	10:i:18:LEU:HD11	2.54	0.42
8:y:107:MET:HE2	8:y:218:ASN:HB3	2.02	0.42
23:y:308:CHL:HBB2	23:y:310:CHL:CBC	2.49	0.42
27:y:319:LHG:H342	27:y:319:LHG:H311	1.91	0.42
19:z:31:ASP:OD1	19:z:34:SER:HB3	2.20	0.42
20:A:184:ILE:O	20:A:328:MET:HE1	2.19	0.42
21:C:216:SER:HB3	21:C:221:GLU:HG3	2.00	0.42
21:c:38:GLY:HA3	24:c:512:CLA:CMD	2.49	0.42
30:c:501:LMG:H232	24:c:504:CLA:C4B	2.50	0.42
24:c:503:CLA:H171	24:c:503:CLA:H13	1.84	0.42
22:r:147:ALA:O	22:r:151:THR:HG22	2.19	0.42
23:9:605:CHL:H3A	23:9:605:CHL:HBA2	1.65	0.42
23:9:608:CHL:H3A	23:9:608:CHL:HBA2	1.37	0.42
2:0:215:LYS:HE2	24:0:611:CLA:C3D	2.49	0.42
2:0:236:LYS:HD2	2:0:240:GLU:OE2	2.19	0.42
3:AB:239:MET:HE3	3:AB:239:MET:O	2.20	0.42
29:AB:313:BCR:H11C	29:AB:313:BCR:H341	1.87	0.42
4:v:18:ARG:NH1	12:Az:5:ASN:HD22	2.17	0.42
24:Au:611:CLA:H62	24:Au:611:CLA:H41	1.82	0.42
4:BE:13:LEU:HD12	4:BE:13:LEU:O	2.19	0.42
24:BE:602:CLA:H111	24:BE:602:CLA:H72	1.74	0.42
7:BI:27:PHE:CD2	29:BI:101:BCR:H14C	2.55	0.42
8:BJ:232:GLN:O	8:BJ:236:THR:HG22	2.20	0.42
24:BJ:602:CLA:HBA2	24:BJ:602:CLA:H12	1.70	0.42
32:BO:101:SQD:H342	32:BO:101:SQD:H312	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BV:196:PHE:HD2	23:BV:607:CHL:HBC3	1.84	0.42
24:BV:609:CLA:H2	25:BV:614:LUT:H28	2.02	0.42
8:Ba:168:LEU:O	8:Ba:172:VAL:HG13	2.20	0.42
8:Ba:250:ASP:OD1	8:Ba:252:VAL:HG22	2.20	0.42
25:Ba:316:LUT:C8	25:Ba:316:LUT:H181	2.48	0.42
21:1:57:ALA:O	21:1:61:VAL:HG23	2.19	0.42
21:1:361:LEU:O	21:1:362:ARG:NH1	2.45	0.42
24:1:513:CLA:H161	24:1:513:CLA:H141	1.66	0.42
20:BD:82:ILE:HB	20:BD:174:LEU:HB2	2.01	0.42
21:BF:272:LEU:O	21:BF:276:LEU:HG	2.19	0.42
27:BU:617:LHG:H202	27:BU:617:LHG:H171	1.79	0.42
28:5:619:XAT:H11	28:5:619:XAT:H191	1.88	0.42
24:D:401:CLA:H41	24:D:401:CLA:H62	1.58	0.42
27:D:404:LHG:H281	27:D:404:LHG:H311	1.92	0.42
8:G:107:MET:HG2	8:G:222:ALA:CB	2.50	0.42
24:N:610:CLA:HBA2	24:N:610:CLA:H3A	1.78	0.42
4:b:392:VAL:HB	4:b:418:LYS:HE2	2.01	0.42
4:b:467:ILE:HD13	4:b:467:ILE:HA	1.76	0.42
5:d:266:ARG:HE	20:a:223:LEU:HD11	1.84	0.42
23:n:607:CHL:H43	23:n:607:CHL:HMA3	2.01	0.42
24:n:611:CLA:H62	24:n:612:CLA:C1D	2.50	0.42
25:n:616:LUT:H15	25:n:616:LUT:H201	1.88	0.42
8:y:175:TYR:HB3	23:y:309:CHL:CMC	2.50	0.42
21:C:272:LEU:O	21:C:276:LEU:HG	2.19	0.42
34:a:401:DGD:HB71	34:a:401:DGD:HBT2	1.71	0.42
22:r:155:LEU:HD12	22:r:155:LEU:HA	1.76	0.42
1:9:162:TRP:CH2	28:9:619:XAT:C13	3.02	0.42
1:9:236:THR:HB	1:9:238:LYS:HZ2	1.85	0.42
24:9:603:CLA:CAD	23:9:609:CHL:H2	2.49	0.42
23:0:606:CHL:HAA1	23:0:606:CHL:CBD	2.50	0.42
1:AA:152:LEU:O	1:AA:154:HIS:N	2.52	0.42
3:AB:126:ALA:HB3	3:AB:129:GLU:CG	2.50	0.42
4:v:243:ALA:HA	4:v:246:PHE:CD2	2.54	0.42
4:v:269:GLY:O	4:v:448:ARG:NH2	2.51	0.42
24:v:609:CLA:H141	24:v:609:CLA:H161	1.79	0.42
24:v:613:CLA:H61	24:v:613:CLA:H41	1.53	0.42
14:A6:105:GLU:OE1	14:A6:105:GLU:N	2.42	0.42
4:BE:151:PHE:HE2	4:BE:203:ILE:HG23	1.85	0.42
5:BG:221:ASN:N	5:BG:221:ASN:HD22	2.17	0.42
8:BJ:105:TRP:HD1	23:BJ:609:CHL:HMD2	1.85	0.42
8:BJ:180:ASN:OD1	8:BJ:181:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BJ:224:PHE:CD2	24:BJ:613:CLA:HAB	2.55	0.42
23:BJ:605:CHL:HBA2	23:BJ:605:CHL:H3A	1.62	0.42
25:BJ:615:LUT:H15	25:BJ:615:LUT:H201	1.88	0.42
25:BJ:616:LUT:H11	25:BJ:616:LUT:H191	1.92	0.42
13:BP:13:LEU:O	13:BP:17:VAL:HG23	2.19	0.42
8:BQ:105:TRP:CD1	23:BQ:609:CHL:HMD3	2.55	0.42
8:BQ:207:ALA:O	8:BQ:211:LEU:HG	2.19	0.42
29:BD:411:BCR:H371	29:BD:411:BCR:H24C	1.80	0.42
23:5:607:CHL:CAA	28:5:619:XAT:H41	2.47	0.42
24:5:614:CLA:CHA	24:5:614:CLA:HBA1	2.50	0.42
3:8:143:GLY:O	22:r:284:ILE:HD11	2.19	0.42
4:B:269:GLY:O	4:B:448:ARG:NH2	2.49	0.42
8:G:106:ALA:CB	8:G:223:MET:HG2	2.50	0.42
8:G:134:ALA:O	8:G:137:GLN:HG2	2.20	0.42
23:N:608:CHL:HBA1	23:N:608:CHL:CBD	2.49	0.42
14:S:122:MET:CE	24:S:609:CLA:HAB	2.41	0.42
14:S:188:TYR:CD1	23:S:607:CHL:CMC	3.03	0.42
24:Y:304:CLA:H3A	24:Y:304:CLA:HBA1	1.80	0.42
4:b:285:TYR:HE2	16:u:88:TYR:HA	1.85	0.42
4:b:384:ARG:HA	4:b:385:ARG:NH1	2.35	0.42
6:e:32:ILE:HD12	6:e:32:ILE:HA	1.89	0.42
10:i:29:GLY:O	10:i:34:ARG:NE	2.52	0.42
8:n:176:ARG:NH2	23:n:609:CHL:O1D	2.52	0.42
8:n:217:LYS:NZ	27:n:618:LHG:O4	2.38	0.42
23:s:606:CHL:C9	23:s:606:CHL:H112	2.50	0.42
19:z:1:MET:HE2	2:0:149:ASN:CB	2.48	0.42
24:A:405:CLA:H142	24:A:405:CLA:H112	1.87	0.42
21:C:378:SER:HA	21:C:381:LYS:HE3	2.01	0.42
20:a:159:LEU:C	20:a:162:PRO:HD2	2.44	0.42
24:c:510:CLA:CAD	24:c:510:CLA:H151	2.50	0.42
24:c:514:CLA:HED2	24:c:514:CLA:HAA1	2.02	0.42
22:r:66:ASP:OD2	22:r:66:ASP:N	2.50	0.42
24:9:603:CLA:H3A	24:9:603:CLA:HBA1	1.81	0.42
28:9:619:XAT:H35	27:0:617:LHG:H161	2.01	0.42
4:v:63:ILE:N	4:v:64:PRO:HD2	2.34	0.42
4:v:153:PHE:HB2	24:v:606:CLA:CBB	2.50	0.42
4:v:173:GLY:HA3	4:v:265:ILE:HD11	2.02	0.42
9:Av:54:LEU:HD23	9:Av:54:LEU:HA	1.92	0.42
23:A6:601:CHL:HBB1	23:A6:601:CHL:CHC	2.44	0.42
8:BB:162:TRP:CH2	8:BB:166:VAL:HG21	2.54	0.42
23:BB:307:CHL:HMC	23:BB:308:CHL:C4C	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BE:606:CLA:HBA2	24:BE:606:CLA:H3A	1.66	0.42
5:BG:140:ARG:HD2	20:BD:225:ARG:NH2	2.35	0.42
14:BV:167:ILE:HG22	14:BV:169:ILE:HG22	2.01	0.42
8:Ba:161:ILE:HA	8:Ba:164:THR:HG22	2.02	0.42
8:Ba:214:LYS:HD2	24:Ba:313:CLA:HBD	2.01	0.42
21:1:451:ALA:HA	21:1:456:GLU:CD	2.45	0.42
24:1:513:CLA:HBA1	24:1:513:CLA:CBD	2.49	0.42
20:BD:37:MET:HE3	20:BD:38:ILE:HG13	2.01	0.42
1:5:105:TRP:CD1	23:5:608:CHL:HED3	2.55	0.42
1:5:119:LEU:HD12	1:5:124:VAL:HG21	2.02	0.42
2:6:111:ILE:HD12	2:6:111:ILE:HA	1.86	0.42
23:6:601:CHL:H141	23:6:601:CHL:H161	1.83	0.42
24:6:602:CLA:H3A	24:6:602:CLA:HBA2	1.42	0.42
1:7:80:TRP:CD1	1:7:80:TRP:C	2.97	0.42
4:B:137:LYS:NZ	9:H:26:LEU:HA	2.35	0.42
29:B:623:BCR:H15C	29:B:623:BCR:H351	1.92	0.42
5:D:133:LEU:O	5:D:137:VAL:HG22	2.19	0.42
6:E:67:THR:HG22	6:E:75:GLN:HE22	1.83	0.42
8:G:223:MET:HE1	24:G:602:CLA:HHC	2.02	0.42
23:G:601:CHL:HED1	27:G:618:LHG:H122	2.02	0.42
8:Y:162:TRP:CH2	8:Y:166:VAL:HG21	2.55	0.42
4:b:472:ARG:HG3	4:b:479:PHE:HE2	1.79	0.42
7:f:27:PHE:CD2	29:f:101:BCR:H14C	2.55	0.42
24:g:603:CLA:H201	27:n:618:LHG:H222	2.02	0.42
25:g:615:LUT:H35	25:g:615:LUT:H401	1.92	0.42
23:n:605:CHL:HAA1	23:n:605:CHL:HBD	2.02	0.42
25:s:615:LUT:H181	25:s:615:LUT:C8	2.50	0.42
16:u:102:ARG:HD2	16:u:103:TYR:H	1.85	0.42
25:y:316:LUT:C8	25:y:316:LUT:H181	2.49	0.42
21:c:120:ILE:HD13	21:c:120:ILE:HA	1.82	0.42
24:c:505:CLA:H3A	24:c:505:CLA:HBA2	1.59	0.42
22:r:159:TRP:CD1	22:r:160:LEU:HD22	2.44	0.42
28:r:616:XAT:H31	28:r:616:XAT:H391	1.82	0.42
2:0:73:GLY:C	24:0:602:CLA:HED3	2.45	0.42
2:0:201:ASP:OD1	2:0:201:ASP:N	2.50	0.42
25:0:615:LUT:H161	25:0:615:LUT:H7	1.87	0.42
1:AA:106:ALA:CB	1:AA:223:MET:HB3	2.48	0.42
24:AB:303:CLA:NB	29:AB:313:BCR:H281	2.35	0.42
24:v:614:CLA:H41	24:v:614:CLA:H62	1.64	0.42
6:3:33:ALA:HA	6:3:36:LEU:HG	2.01	0.42
24:BB:314:CLA:C1B	24:BB:315:CLA:HMD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:26:ASP:OD2	5:BG:26:ASP:C	2.63	0.42
5:BG:243:GLU:HG3	20:BD:244:GLU:CD	2.45	0.42
8:BJ:165:GLN:HG3	23:BJ:606:CHL:HMA3	2.02	0.42
8:BJ:226:MET:HB3	8:BJ:226:MET:HE2	1.40	0.42
24:BJ:604:CLA:CMB	23:BJ:606:CHL:HBB1	2.50	0.42
10:BL:16:VAL:O	10:BL:20:ILE:HG22	2.20	0.42
14:BV:103:LYS:HB2	14:BV:106:ASN:HB2	2.02	0.42
17:BY:86:SER:O	17:BY:86:SER:OG	2.37	0.42
24:Ba:303:CLA:H91	24:Ba:303:CLA:H111	1.82	0.42
24:1:508:CLA:H161	24:1:508:CLA:H141	1.67	0.42
24:1:513:CLA:HBD	24:1:513:CLA:HED3	1.78	0.42
24:BF:511:CLA:H193	24:BF:511:CLA:H162	1.89	0.42
22:BU:148:MET:SD	22:BU:148:MET:C	3.03	0.42
24:5:603:CLA:C2D	23:5:609:CHL:H52	2.49	0.41
24:6:614:CLA:HBC2	27:6:617:LHG:H351	2.02	0.41
24:7:305:CLA:H3A	24:7:305:CLA:HBA2	1.39	0.41
4:B:155:ALA:O	4:B:159:THR:OG1	2.36	0.41
5:D:196:PRO:HD3	12:L:35:TYR:CE2	2.55	0.41
5:D:266:ARG:NH2	5:D:270:PHE:HB2	2.34	0.41
24:b:609:CLA:H62	24:b:609:CLA:H92	1.71	0.41
8:g:140:SER:OG	8:g:143:GLY:O	2.37	0.41
8:g:232:GLN:O	8:g:236:THR:HG22	2.20	0.41
8:g:237:GLY:C	8:g:238:LYS:HD2	2.45	0.41
11:k:50:LEU:O	11:k:53:VAL:HG12	2.19	0.41
8:n:216:LEU:HD12	8:n:216:LEU:HA	1.89	0.41
8:n:229:PHE:HE1	25:n:615:LUT:H41	1.85	0.41
23:y:306:CHL:HAA1	23:y:306:CHL:HBD	2.02	0.41
25:y:316:LUT:H35	25:y:316:LUT:H401	1.91	0.41
29:z:101:BCR:H23C	24:c:514:CLA:H122	2.02	0.41
29:z:102:BCR:H24C	29:z:102:BCR:H371	1.87	0.41
21:c:162:GLY:HA2	21:c:248:GLY:HA2	2.01	0.41
21:c:269:GLU:OE2	21:c:444:HIS:ND1	2.38	0.41
27:r:618:LHG:H171	27:r:618:LHG:H202	1.82	0.41
3:AB:170:GLN:HG3	23:AB:306:CHL:HMC	2.01	0.41
24:v:603:CLA:CGA	24:v:603:CLA:H3A	2.49	0.41
8:Au:57:LYS:HB2	8:Au:63:SER:OG	2.20	0.41
9:Av:19:VAL:O	9:Av:23:LEU:HG	2.20	0.41
4:BE:25:MET:HE1	29:BE:618:BCR:C23	2.49	0.41
5:BG:157:VAL:HG13	5:BG:158:PHE:CD1	2.55	0.41
5:BG:266:ARG:HH12	20:BD:237:TYR:N	2.17	0.41
23:BJ:607:CHL:H143	23:BJ:607:CHL:H111	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BQ:226:MET:SD	25:BQ:616:LUT:H12	2.60	0.41
23:BV:605:CHL:HMC	23:BV:606:CHL:C1C	2.50	0.41
25:BV:614:LUT:C8	25:BV:614:LUT:H181	2.50	0.41
23:Ba:302:CHL:H3A	23:Ba:302:CHL:HBA1	1.60	0.41
23:Ba:310:CHL:HBC3	23:Ba:310:CHL:HMC	2.02	0.41
24:Ba:311:CLA:H102	24:Ba:311:CLA:H13	1.77	0.41
20:BD:235:GLU:OE1	20:BD:235:GLU:HA	2.19	0.41
24:BF:509:CLA:CBB	24:BF:510:CLA:HED1	2.50	0.41
2:6:215:LYS:HE2	24:6:611:CLA:C3D	2.50	0.41
23:6:606:CHL:HBB2	23:6:607:CHL:CBB	2.45	0.41
3:8:102:GLU:OE2	3:8:233:ARG:NE	2.38	0.41
24:B:602:CLA:H62	24:B:602:CLA:H41	1.75	0.41
24:B:613:CLA:H91	24:B:613:CLA:H111	1.62	0.41
8:G:57:LYS:HB2	8:G:63:SER:OG	2.20	0.41
23:Y:302:CHL:H202	23:Y:302:CHL:H161	1.73	0.41
25:Y:317:LUT:H31	25:Y:317:LUT:H391	1.94	0.41
4:b:453:PHE:HB2	5:d:292:LEU:HD12	2.02	0.41
5:d:121:PHE:HA	5:d:124:ILE:CG2	2.50	0.41
24:g:604:CLA:CMB	23:g:606:CHL:HBB1	2.50	0.41
24:g:604:CLA:HBA1	23:g:606:CHL:CHD	2.51	0.41
8:n:231:VAL:HG11	24:n:613:CLA:CAC	2.45	0.41
24:n:613:CLA:H61	24:n:613:CLA:H2	1.82	0.41
14:s:106:ASN:HB3	14:s:110:TYR:CE1	2.56	0.41
14:s:224:LYS:HE2	24:s:611:CLA:HBD	2.00	0.41
30:C:501:LMG:H212	24:C:504:CLA:C2B	2.49	0.41
24:C:509:CLA:H142	24:C:509:CLA:H112	1.78	0.41
24:c:509:CLA:H2	24:c:511:CLA:H12	2.01	0.41
22:r:183:PRO:O	22:r:184:LEU:HD13	2.20	0.41
2:0:112:THR:O	2:0:116:LEU:HD22	2.19	0.41
2:0:209:LEU:CD2	24:0:610:CLA:H3A	2.48	0.41
24:AA:305:CLA:C1B	26:AA:319:NEX:H383	2.49	0.41
3:AB:126:ALA:HB3	3:AB:129:GLU:HG2	2.00	0.41
3:AB:174:TRP:CE2	22:BU:56:PRO:HA	2.55	0.41
5:2:270:PHE:HZ	27:2:405:LHG:HC5	1.84	0.41
5:2:290:LEU:HD23	5:2:290:LEU:HA	1.86	0.41
5:BG:242:GLU:OE1	5:BG:242:GLU:N	2.53	0.41
8:BJ:226:MET:HE1	25:BJ:616:LUT:C12	2.20	0.41
23:BQ:601:CHL:H41	23:BQ:601:CHL:H62	1.67	0.41
16:BX:82:GLU:O	16:BX:86:LYS:HG2	2.20	0.41
8:Ba:55:ARG:O	8:Ba:57:LYS:NZ	2.53	0.41
8:Ba:111:LEU:HA	8:Ba:114:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BU:80:PRO:HG2	22:BU:81:PHE:HD1	1.83	0.41
22:BU:240:LEU:HD12	22:BU:240:LEU:O	2.20	0.41
22:BU:250:MET:HE2	24:BU:602:CLA:CMC	2.49	0.41
3:8:83:PHE:HE2	28:8:312:XAT:H383	1.84	0.41
24:8:301:CLA:H3A	24:8:301:CLA:HBA2	1.35	0.41
4:B:55:MET:HE2	4:B:55:MET:HB3	1.77	0.41
24:B:609:CLA:H141	24:B:609:CLA:H161	1.80	0.41
24:B:609:CLA:HMA2	24:B:610:CLA:C2C	2.50	0.41
5:D:176:VAL:HG21	24:A:407:CLA:HED1	2.02	0.41
5:D:200:MET:CE	5:D:282:MET:HG2	2.41	0.41
5:D:216:GLY:HA3	20:A:276:ALA:HB2	2.02	0.41
5:D:266:ARG:NH2	20:A:220:THR:OG1	2.40	0.41
8:G:152:LEU:O	8:G:154:HIS:N	2.53	0.41
23:G:601:CHL:C10	23:G:601:CHL:H61	2.50	0.41
14:S:129:ILE:HD13	14:S:129:ILE:HA	1.90	0.41
4:b:224:ARG:H	4:b:224:ARG:HG2	1.58	0.41
6:e:52:PRO:HB3	7:f:39:ARG:HG3	2.02	0.41
25:g:615:LUT:H181	25:g:615:LUT:C8	2.50	0.41
8:n:73:GLU:HG3	8:n:74:PHE:CD2	2.55	0.41
23:n:606:CHL:HBA1	23:n:606:CHL:H3A	1.84	0.41
14:s:103:LYS:HB2	14:s:106:ASN:HB2	2.01	0.41
8:y:80:TRP:HD1	8:y:82:THR:HG23	1.85	0.41
24:a:410:CLA:H111	24:a:410:CLA:H91	1.82	0.41
22:r:271:TRP:CD1	22:r:275:LEU:HD23	2.55	0.41
23:9:607:CHL:HMA1	23:9:607:CHL:HHB	1.81	0.41
24:9:610:CLA:H92	24:9:610:CLA:H61	1.80	0.41
2:0:230:GLN:O	2:0:234:THR:HG22	2.20	0.41
3:AB:143:GLY:O	22:BU:284:ILE:HD11	2.20	0.41
7:4:27:PHE:O	7:4:31:ILE:HG12	2.20	0.41
24:Au:602:CLA:H142	24:Au:602:CLA:H111	1.75	0.41
23:Au:607:CHL:H191	23:A2:601:CHL:H41	2.01	0.41
13:A1:8:PHE:HD2	13:A1:8:PHE:O	2.03	0.41
23:A2:608:CHL:H12	23:A2:608:CHL:H51	1.66	0.41
14:A6:80:GLU:OE2	19:BC:37:LYS:NZ	2.53	0.41
8:BB:226:MET:HE3	8:BB:229:PHE:HB2	2.02	0.41
19:BC:46:LEU:O	19:BC:50:LEU:HG	2.21	0.41
4:BE:155:ALA:O	4:BE:159:THR:OG1	2.26	0.41
5:BG:56:VAL:O	5:BG:67:SER:HB3	2.20	0.41
6:BH:42:LEU:O	6:BH:46:VAL:HG12	2.20	0.41
8:BJ:152:LEU:HA	23:BJ:605:CHL:HED2	2.02	0.41
24:1:507:CLA:H2	24:1:507:CLA:HMA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BD:411:BCR:H15C	29:BD:411:BCR:H351	1.87	0.41
21:BF:60:ILE:HD13	24:BF:511:CLA:HMC1	2.02	0.41
21:BF:142:GLU:OE1	21:BF:143:SER:OG	2.29	0.41
21:BF:228:ASP:OD1	21:BF:228:ASP:N	2.52	0.41
24:BF:513:CLA:H91	24:BF:513:CLA:H112	1.70	0.41
24:BU:603:CLA:H91	24:BU:603:CLA:H112	1.83	0.41
28:5:619:XAT:H11	24:6:613:CLA:H41	2.02	0.41
2:6:221:MET:HE1	24:6:602:CLA:CHC	2.45	0.41
1:7:110:ALA:O	1:7:114:VAL:HG12	2.21	0.41
23:8:304:CHL:H3A	29:8:313:BCR:H21C	2.02	0.41
29:B:618:BCR:H24C	29:B:618:BCR:H371	1.90	0.41
5:D:111:LEU:HD23	5:D:111:LEU:HA	1.86	0.41
5:D:280:LEU:HG	38:A:409:PHO:HBC3	2.01	0.41
24:N:614:CLA:HHC	24:N:614:CLA:CBB	2.47	0.41
24:S:602:CLA:H102	25:S:615:LUT:H371	2.02	0.41
16:U:102:ARG:HG2	16:U:103:TYR:H	1.84	0.41
8:Y:105:TRP:CD1	23:Y:310:CHL:HMD2	2.56	0.41
8:Y:214:LYS:HE2	24:Y:312:CLA:HED1	2.03	0.41
5:d:174:PHE:N	5:d:174:PHE:HD1	2.18	0.41
24:s:603:CLA:HBA1	24:s:603:CLA:H3A	1.79	0.41
25:s:615:LUT:H11	25:s:615:LUT:H191	1.95	0.41
8:y:250:ASP:OD1	8:y:252:VAL:HG22	2.19	0.41
38:A:409:PHO:H71	38:A:409:PHO:H112	1.78	0.41
21:C:57:ALA:O	21:C:61:VAL:HG23	2.20	0.41
21:C:447:ARG:HD3	24:C:508:CLA:HED2	2.02	0.41
24:C:506:CLA:O1A	24:C:506:CLA:H3A	2.20	0.41
22:r:76:TYR:CD1	24:r:601:CLA:HAC1	2.55	0.41
22:r:209:GLU:CD	22:r:215:ARG:HG2	2.45	0.41
22:r:233:GLU:O	22:r:237:GLN:HG2	2.21	0.41
22:r:240:LEU:HD12	22:r:240:LEU:O	2.21	0.41
24:r:609:CLA:H172	25:r:615:LUT:H391	2.02	0.41
1:9:165:GLN:HG3	23:9:606:CHL:HMA3	2.03	0.41
24:0:614:CLA:HBC2	27:0:617:LHG:H351	2.02	0.41
1:AA:75:PRO:HD2	1:AA:96:ARG:NH2	2.35	0.41
24:AA:303:CLA:H3A	24:AA:303:CLA:O1A	2.21	0.41
3:AB:222:GLU:HA	3:AB:225:LYS:HD2	2.02	0.41
4:v:419:LYS:NZ	4:v:420:TYR:CD1	2.88	0.41
24:v:615:CLA:H8	24:v:615:CLA:H52	1.91	0.41
5:2:176:VAL:HG21	24:R:406:CLA:HED1	2.02	0.41
23:Au:601:CHL:H18	23:BB:308:CHL:H121	2.03	0.41
8:A2:128:GLU:O	8:A2:137:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A2:186:ALA:HB2	23:A2:608:CHL:HBC1	2.01	0.41
25:A6:615:LUT:H35	25:A6:615:LUT:H401	1.92	0.41
4:BE:151:PHE:CE2	4:BE:207:THR:HG22	2.55	0.41
4:BE:237:VAL:HG23	24:BE:613:CLA:HMD3	2.02	0.41
29:BE:620:BCR:H15C	29:BE:620:BCR:H351	1.92	0.41
25:BJ:615:LUT:C8	25:BJ:615:LUT:H181	2.49	0.41
8:BQ:172:VAL:HA	8:BQ:175:TYR:CD1	2.55	0.41
14:BV:146:VAL:O	14:BV:150:THR:HG23	2.19	0.41
25:BV:615:LUT:H181	25:BV:615:LUT:C8	2.50	0.41
23:Ba:309:CHL:H41	23:Ba:309:CHL:H62	1.83	0.41
20:R:310:GLN:HG3	20:R:310:GLN:O	2.20	0.41
24:R:404:CLA:H72	24:R:404:CLA:H111	1.80	0.41
21:BF:396:MET:SD	21:BF:397:THR:N	2.94	0.41
1:5:107:MET:HE2	24:5:610:CLA:CMC	2.48	0.41
2:6:75:TYR:OH	27:6:617:LHG:O5	2.28	0.41
24:6:604:CLA:H3A	24:6:604:CLA:HBA2	1.30	0.41
24:6:604:CLA:HHD	24:6:604:CLA:HAC2	1.78	0.41
4:B:198:ILE:HD12	4:B:198:ILE:H	1.86	0.41
5:D:173:SER:HB3	5:D:178:ALA:HB1	2.02	0.41
5:D:344:GLU:OE2	5:D:349:ARG:HD2	2.21	0.41
8:G:214:LYS:NZ	24:G:611:CLA:HBD	2.35	0.41
25:G:615:LUT:H15	25:G:615:LUT:H201	1.91	0.41
23:Y:306:CHL:HAA1	23:Y:306:CHL:CBD	2.50	0.41
19:Z:19:LEU:O	19:Z:23:VAL:HG23	2.19	0.41
4:b:460:LEU:HD23	5:d:285:LEU:HD12	2.02	0.41
24:b:609:CLA:H91	24:b:609:CLA:H111	1.65	0.41
24:d:402:CLA:H91	24:d:402:CLA:H112	1.70	0.41
23:g:601:CHL:HHC	23:g:601:CHL:HBB1	2.01	0.41
8:y:191:TYR:HB3	24:y:311:CLA:HED2	2.02	0.41
25:y:316:LUT:H31	25:y:316:LUT:H391	1.94	0.41
25:y:317:LUT:H31	25:y:317:LUT:H391	1.92	0.41
20:A:24:THR:OG1	20:A:25:GLU:OE2	2.31	0.41
21:C:33:PHE:O	21:C:41:ARG:NH2	2.41	0.41
21:c:63:TRP:CE2	21:c:67:MET:HG3	2.55	0.41
21:c:168:LEU:HD11	24:c:508:CLA:HED2	2.01	0.41
21:c:230:LEU:O	21:c:234:ILE:HG12	2.21	0.41
24:0:602:CLA:H52	25:0:616:LUT:H28	2.02	0.41
24:AA:311:CLA:H3A	24:AA:311:CLA:CGA	2.50	0.41
4:v:215:PHE:CZ	24:v:609:CLA:HMD2	2.54	0.41
24:v:602:CLA:H102	24:v:609:CLA:H193	2.02	0.41
8:Au:134:ALA:O	8:Au:137:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Au:616:LUT:H31	25:Au:616:LUT:H391	1.94	0.41
29:Ay:102:BCR:H373	21:1:55:ALA:HB1	2.01	0.41
13:A1:27:VAL:CG1	13:BP:28:LYS:HB2	2.51	0.41
8:A2:128:GLU:C	8:A2:128:GLU:CD	2.89	0.41
30:A0:201:LMG:H372	30:A0:201:LMG:H341	1.71	0.41
8:BJ:109:GLY:HA2	25:BJ:616:LUT:H181	2.03	0.41
23:BJ:601:CHL:OBD	24:BJ:602:CLA:HHD	2.21	0.41
23:BJ:608:CHL:HBA1	23:BJ:608:CHL:H192	2.03	0.41
11:BN:34:ASN:O	11:BN:37:VAL:HG12	2.20	0.41
8:BQ:155:ALA:HA	23:BQ:605:CHL:CHC	2.50	0.41
8:BQ:241:ILE:H	8:BQ:241:ILE:HG13	1.63	0.41
24:BQ:610:CLA:H111	24:BQ:610:CLA:H72	1.79	0.41
14:BV:187:TYR:O	14:BV:191:THR:OG1	2.30	0.41
23:BV:606:CHL:C9	23:BV:606:CHL:H112	2.51	0.41
23:Ba:310:CHL:C9	23:Ba:310:CHL:H112	2.50	0.41
19:Bb:33:TRP:HZ3	19:Bb:40:VAL:HG21	1.85	0.41
34:1:518:DGD:HAE2	34:1:518:DGD:HA82	1.83	0.41
24:BF:509:CLA:HBC3	24:BF:511:CLA:H92	2.02	0.41
24:BF:514:CLA:HBA1	24:BF:514:CLA:CHA	2.51	0.41
2:6:179:ASP:N	14:BV:102:LYS:HD2	2.35	0.41
25:6:615:LUT:H161	25:6:615:LUT:H7	1.78	0.41
3:8:98:TYR:CD1	24:8:301:CLA:HHB	2.55	0.41
5:D:285:LEU:HD23	5:D:285:LEU:HA	1.86	0.41
5:D:322:LEU:HD13	20:A:184:ILE:CG2	2.51	0.41
25:S:614:LUT:H181	25:S:614:LUT:C8	2.50	0.41
16:U:102:ARG:HG2	16:U:103:TYR:N	2.36	0.41
23:Y:310:CHL:H192	23:Y:310:CHL:H161	1.76	0.41
4:b:385:ARG:H	4:b:385:ARG:NE	2.19	0.41
24:b:616:CLA:H91	24:b:616:CLA:H111	1.66	0.41
5:d:174:PHE:N	5:d:174:PHE:CD1	2.88	0.41
25:s:614:LUT:H35	25:s:614:LUT:H401	1.94	0.41
22:r:282:THR:HB	23:r:613:CHL:HED1	2.01	0.41
23:AB:306:CHL:HBA2	23:AB:306:CHL:H3A	1.39	0.41
24:v:615:CLA:H93	24:v:615:CLA:H111	1.71	0.41
23:Au:608:CHL:H143	23:Au:608:CHL:H162	1.70	0.41
24:A6:602:CLA:CBB	25:A6:615:LUT:H32	2.51	0.41
16:A8:102:ARG:HG2	16:A8:103:TYR:N	2.36	0.41
8:BB:105:TRP:HD1	23:BB:310:CHL:HMD2	1.86	0.41
23:BB:308:CHL:H203	23:BB:308:CHL:H161	1.74	0.41
24:BE:604:CLA:H193	24:BE:604:CLA:H162	1.82	0.41
24:BE:609:CLA:HAA1	24:BE:609:CLA:HED2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BO:25:ILE:HD13	12:BO:25:ILE:HA	1.84	0.41
12:BO:26:PHE:O	12:BO:30:VAL:HG12	2.20	0.41
8:BQ:229:PHE:HE1	25:BQ:615:LUT:H41	1.86	0.41
14:BV:222:LYS:HD3	24:BV:609:CLA:HMA3	2.01	0.41
20:R:204:GLY:HA2	20:R:278:TRP:HE1	1.86	0.41
24:1:506:CLA:H43	29:1:515:BCR:H323	2.02	0.41
24:BD:410:CLA:H91	24:BD:410:CLA:H111	1.82	0.41
30:BF:501:LMG:H232	24:BF:504:CLA:C4B	2.50	0.41
24:BU:602:CLA:H111	24:BU:602:CLA:H93	1.76	0.41
24:BU:603:CLA:C1D	24:BU:608:CLA:H62	2.50	0.41
23:BU:605:CHL:CMC	23:BU:606:CHL:C4C	2.99	0.41
2:6:91:LYS:HZ1	1:7:83:ALA:HA	1.86	0.41
3:8:91:ASP:HB3	3:8:94:PHE:HB2	2.03	0.41
4:B:18:ARG:HD3	4:B:115:TRP:CZ3	2.56	0.41
4:B:105:GLY:O	4:B:108:PHE:HB3	2.21	0.41
7:F:22:VAL:HB	7:F:23:PRO:HD3	2.01	0.41
23:G:609:CHL:HBB1	23:G:609:CHL:CHC	2.51	0.41
13:M:1:MET:HG3	13:M:3:VAL:HG23	2.02	0.41
13:M:8:PHE:C	13:M:8:PHE:CD2	2.97	0.41
13:M:27:VAL:CG1	13:m:28:LYS:HB2	2.51	0.41
24:b:616:CLA:HBA1	24:b:616:CLA:H3A	1.89	0.41
29:b:619:BCR:H20C	29:b:619:BCR:H361	1.93	0.41
5:d:176:VAL:HG22	24:a:407:CLA:HED1	2.03	0.41
24:g:613:CLA:H2	24:g:613:CLA:H61	1.76	0.41
8:n:155:ALA:HA	23:n:605:CHL:CHC	2.51	0.41
24:n:602:CLA:H161	24:n:602:CLA:H141	1.86	0.41
23:n:606:CHL:HAA1	23:n:606:CHL:CGD	2.51	0.41
25:s:614:LUT:C8	25:s:614:LUT:H181	2.50	0.41
29:z:101:BCR:H24C	29:z:101:BCR:H371	1.86	0.41
24:C:507:CLA:H93	24:C:507:CLA:H112	1.82	0.41
24:c:514:CLA:HBA1	24:c:514:CLA:CHA	2.51	0.41
24:r:611:CLA:HHC	24:r:611:CLA:HBB1	2.01	0.41
2:0:62:GLN:OE1	2:0:62:GLN:N	2.52	0.41
2:0:221:MET:HG3	25:0:616:LUT:C35	2.50	0.41
1:AA:204:ASP:HB3	1:AA:207:ALA:HB3	2.02	0.41
3:AB:201:ASP:OD1	24:AB:308:CLA:HBD	2.21	0.41
23:AB:304:CHL:CBD	23:AB:304:CHL:HAA1	2.51	0.41
24:v:602:CLA:H101	9:Av:58:LEU:HD12	2.02	0.41
24:v:605:CLA:H41	24:v:605:CLA:H62	1.50	0.41
24:v:608:CLA:H92	24:v:608:CLA:H62	1.72	0.41
8:Au:170:GLY:CA	23:Au:609:CHL:HAB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Av:102:DGD:HB51	34:Av:102:DGD:HB81	1.69	0.41
24:A2:611:CLA:H2A	24:A2:611:CLA:O1D	2.21	0.41
8:BB:229:PHE:CE1	25:BB:316:LUT:H41	2.55	0.41
24:BB:312:CLA:HBA2	24:BB:312:CLA:H3A	1.49	0.41
5:BG:322:LEU:HD23	20:BD:331:MET:HB3	2.02	0.41
6:BH:32:ILE:O	6:BH:36:LEU:HD22	2.20	0.41
8:BJ:140:SER:OG	8:BJ:143:GLY:O	2.37	0.41
10:BL:3:THR:H	10:BL:3:THR:HG23	1.64	0.41
23:BQ:606:CHL:HAA1	23:BQ:606:CHL:CGD	2.51	0.41
25:BQ:615:LUT:H35	25:BQ:615:LUT:H401	1.91	0.41
21:1:168:LEU:HD13	24:1:507:CLA:H43	2.01	0.41
20:BD:286:THR:O	20:BD:290:ILE:HG22	2.21	0.41
24:BF:514:CLA:HAA1	24:BF:514:CLA:HED2	2.03	0.41
29:BF:515:BCR:H20C	29:BF:515:BCR:H361	1.80	0.41
22:BU:205:GLN:NE2	23:BU:607:CHL:C2C	2.83	0.41
22:BU:231:ASP:OD2	22:BU:233:GLU:HG3	2.20	0.41
24:BU:609:CLA:H141	24:BU:609:CLA:H162	1.83	0.41
1:5:234:ILE:HD12	1:5:234:ILE:HA	1.82	0.41
25:6:616:LUT:H35	25:6:616:LUT:H401	1.90	0.41
4:B:208:LEU:HD12	4:B:208:LEU:HA	1.86	0.41
24:B:605:CLA:H111	24:B:605:CLA:H91	1.82	0.41
8:G:110:ALA:HB1	25:G:615:LUT:H12	2.02	0.41
23:G:607:CHL:H121	23:N:601:CHL:H201	2.03	0.41
10:I:8:VAL:HG21	20:A:97:TRP:CZ3	2.55	0.41
24:S:602:CLA:H62	24:S:602:CLA:H41	1.79	0.41
23:Y:307:CHL:HMC	23:Y:308:CHL:C1C	2.50	0.41
5:d:234:ARG:NH1	32:d:406:SQD:H61	2.35	0.41
9:h:54:LEU:HD23	9:h:54:LEU:HA	1.86	0.41
25:n:615:LUT:H31	25:n:615:LUT:H391	1.94	0.41
8:y:165:GLN:HG3	23:y:307:CHL:HMA3	2.03	0.41
29:z:101:BCR:H381	24:c:514:CLA:H11	2.02	0.41
24:C:502:CLA:HBA2	24:C:502:CLA:H3A	1.14	0.41
20:a:99:ALA:HB3	20:a:105:TRP:HB2	2.03	0.41
22:r:209:GLU:OE2	22:r:214:LYS:HB3	2.21	0.41
24:r:612:CLA:HMA1	25:r:615:LUT:H22	2.02	0.41
23:9:609:CHL:HBC3	23:9:609:CHL:HMC	2.01	0.41
2:0:156:ILE:CG1	2:0:160:LEU:HD21	2.51	0.41
2:0:172:GLY:CA	1:AA:62:PHE:CE1	2.86	0.41
2:0:215:LYS:HZ3	24:0:611:CLA:CGD	2.33	0.41
25:AA:316:LUT:H161	25:AA:316:LUT:H7	1.83	0.41
3:AB:224:LEU:HG	3:AB:224:LEU:H	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:603:CLA:C3D	24:v:605:CLA:H43	2.51	0.41
24:v:614:CLA:H141	24:v:614:CLA:H161	1.63	0.41
8:Au:223:MET:HE1	24:Au:602:CLA:CAB	2.51	0.41
24:Aw:102:CLA:H161	24:Aw:102:CLA:H192	1.78	0.41
8:BB:105:TRP:CD1	23:BB:310:CHL:HMD2	2.56	0.41
24:BE:608:CLA:H2	30:BE:621:LMG:H151	2.03	0.41
5:BG:19:MET:CE	18:BZ:103:VAL:HA	2.51	0.41
5:BG:211:LEU:HD21	31:BG:403:PL9:H172	2.02	0.41
8:BJ:247:HIS:HD1	8:BJ:251:PRO:HA	1.86	0.41
24:BJ:611:CLA:H2A	24:BJ:611:CLA:O1D	2.21	0.41
25:BJ:615:LUT:H35	25:BJ:615:LUT:H401	1.92	0.41
10:BL:31:ASN:OD1	10:BL:31:ASN:C	2.63	0.41
24:Ba:312:CLA:HBA2	24:Ba:312:CLA:H3A	1.60	0.41
25:Ba:316:LUT:H15	25:Ba:316:LUT:H201	1.93	0.41
21:BF:363:ALA:O	21:BF:367:GLU:HG2	2.21	0.41
24:BF:510:CLA:H142	24:BF:510:CLA:H112	1.83	0.41
1:5:171:ALA:O	1:5:175:TYR:HD1	2.04	0.41
1:5:209:ALA:HA	1:5:212:LYS:HD2	2.03	0.41
24:5:603:CLA:CAD	23:5:609:CHL:H2	2.50	0.41
2:6:71:PHE:CE2	2:6:93:ARG:NH1	2.89	0.41
2:6:89:PHE:CD1	2:6:93:ARG:NH2	2.89	0.41
24:6:613:CLA:HBA2	24:6:613:CLA:H3A	1.96	0.41
1:7:144:LEU:HD12	1:7:144:LEU:HA	1.83	0.41
3:8:146:LEU:HD23	3:8:150:LEU:HD21	2.03	0.41
4:B:138:ILE:HD13	4:B:138:ILE:HA	1.92	0.41
4:B:247:PHE:CE1	24:B:602:CLA:H122	2.55	0.41
24:B:601:CLA:HBA2	24:B:601:CLA:H3A	1.66	0.41
32:D:406:SQD:H111	32:D:406:SQD:H142	1.53	0.41
8:G:216:LEU:HA	8:G:216:LEU:HD23	1.82	0.41
8:G:237:GLY:C	8:G:238:LYS:HD3	2.46	0.41
23:G:607:CHL:H192	23:G:607:CHL:H161	1.93	0.41
34:H:102:DGD:HBW2	34:H:102:DGD:HB91	1.82	0.41
13:M:18:PRO:O	13:M:22:LEU:HG	2.21	0.41
8:N:128:GLU:O	8:N:137:GLN:NE2	2.54	0.41
8:N:241:ILE:HD13	8:N:241:ILE:HA	1.94	0.41
14:S:170:ASN:OD1	14:S:173:LEU:HD13	2.21	0.41
24:Y:304:CLA:H92	24:Y:304:CLA:H61	1.78	0.41
4:b:54:PRO:HD2	4:b:57:ARG:HG3	2.03	0.41
4:b:155:ALA:O	4:b:159:THR:OG1	2.27	0.41
24:b:610:CLA:H3A	24:b:610:CLA:HBA2	1.31	0.41
29:b:619:BCR:HC42	30:b:621:LMG:H362	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:91:LEU:HD23	5:d:110:GLY:HA2	2.02	0.41
8:g:101:ILE:HD12	8:g:101:ILE:HA	1.91	0.41
8:g:229:PHE:CE1	25:g:615:LUT:H41	2.56	0.41
23:g:606:CHL:C3	26:g:617:NEX:H35	2.51	0.41
9:h:50:PHE:HD2	9:h:50:PHE:O	2.04	0.41
29:h:101:BCR:H371	29:h:101:BCR:H24C	1.81	0.41
12:l:12:GLU:OE2	12:l:12:GLU:N	2.54	0.41
13:m:6:LEU:HA	13:m:9:ILE:HD13	2.03	0.41
8:n:172:VAL:HA	8:n:175:TYR:CD1	2.56	0.41
14:s:237:LEU:O	14:s:241:ILE:HG22	2.21	0.41
16:u:100:ILE:H	16:u:100:ILE:HG12	1.72	0.41
8:y:152:LEU:O	8:y:154:HIS:N	2.53	0.41
24:y:311:CLA:H102	24:y:311:CLA:H13	1.74	0.41
29:z:101:BCR:H20C	29:z:101:BCR:H361	1.80	0.41
24:A:410:CLA:H91	24:A:410:CLA:H111	1.81	0.41
21:C:429:SER:O	21:C:433:LEU:HD23	2.21	0.41
20:a:200:LEU:HD22	20:a:285:PHE:CD1	2.56	0.41
21:c:138:GLU:H	21:c:138:GLU:CD	2.19	0.41
24:r:609:CLA:H162	24:r:609:CLA:H141	1.83	0.41
27:r:618:LHG:H122	27:r:618:LHG:H151	1.84	0.41
24:9:613:CLA:H72	28:AA:301:XAT:H203	2.03	0.41
24:9:614:CLA:CHA	24:9:614:CLA:HBA1	2.50	0.41
25:9:616:LUT:H35	25:9:616:LUT:H401	1.89	0.41
1:AA:62:PHE:HD2	1:AA:62:PHE:HA	1.58	0.41
28:AA:318:XAT:H201	28:AA:318:XAT:H15	1.83	0.41
3:AB:108:TRP:HD1	23:AB:307:CHL:HMD3	1.82	0.41
3:AB:120:GLN:NE2	3:AB:126:ALA:HA	2.36	0.41
3:AB:237:VAL:O	3:AB:241:ILE:HG22	2.21	0.41
4:v:18:ARG:HD3	4:v:115:TRP:CZ3	2.55	0.41
4:v:224:ARG:HH22	9:Av:37:TRP:CA	2.26	0.41
5:2:90:LEU:HG	9:Av:62:ASN:ND2	2.34	0.41
5:2:216:GLY:HA3	20:R:276:ALA:HB2	2.02	0.41
5:2:266:ARG:NH1	20:R:220:THR:CG2	2.83	0.41
8:Au:78:TYR:HE2	23:Au:601:CHL:HBC2	1.85	0.41
8:Au:107:MET:HG2	8:Au:222:ALA:CB	2.51	0.41
23:Au:608:CHL:H3A	23:Au:608:CHL:HBA2	1.44	0.41
24:Au:611:CLA:HBA1	24:Au:611:CLA:H3A	1.94	0.41
23:A2:606:CHL:CBB	25:A2:616:LUT:H161	2.48	0.41
23:A2:607:CHL:C9	23:A2:607:CHL:C11	2.99	0.41
14:A6:67:ARG:CZ	14:A6:92:ASP:OD1	2.68	0.41
26:A6:616:NEX:C10	26:A6:616:NEX:H181	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:306:CHL:HAA1	23:BB:306:CHL:CBD	2.51	0.41
23:BB:309:CHL:H193	23:BB:309:CHL:H161	1.87	0.41
24:BB:314:CLA:H3A	24:BB:314:CLA:HBA2	1.70	0.41
26:BB:318:NEX:H11	26:BB:318:NEX:H191	1.98	0.41
4:BE:18:ARG:NH1	12:BO:5:ASN:HD22	2.18	0.41
4:BE:467:ILE:HA	4:BE:467:ILE:HD13	1.75	0.41
24:BE:602:CLA:H142	24:BE:602:CLA:H112	1.66	0.41
24:BE:616:CLA:H2	24:BE:616:CLA:H61	1.71	0.41
5:BG:273:LEU:HD12	20:BD:217:SER:HB2	2.03	0.41
24:BG:402:CLA:H91	24:BG:402:CLA:H112	1.70	0.41
8:BJ:237:GLY:C	8:BJ:238:LYS:HD2	2.45	0.41
24:BJ:603:CLA:H201	27:BQ:618:LHG:H222	2.03	0.41
25:BJ:616:LUT:H15	25:BJ:616:LUT:H201	1.94	0.41
12:BO:12:GLU:HA	13:BP:29:THR:HG21	2.02	0.41
12:BO:15:ARG:NH1	32:BO:101:SQD:H462	2.36	0.41
8:BQ:240:PRO:HA	8:BQ:243:ASN:HD22	1.86	0.41
23:BQ:607:CHL:HBA1	23:BQ:607:CHL:H3A	1.52	0.41
14:BV:195:ASP:O	14:BV:195:ASP:CG	2.63	0.41
24:BV:609:CLA:H41	24:BV:609:CLA:H62	1.84	0.41
21:1:36:TRP:O	24:1:508:CLA:H42	2.21	0.41
21:1:223:TRP:CG	21:1:224:ILE:H	2.39	0.41
20:BD:223:LEU:HA	20:BD:223:LEU:HD12	1.83	0.41
24:BF:504:CLA:H172	24:BF:511:CLA:HBB2	2.02	0.41
30:BF:519:LMG:H132	30:BF:519:LMG:HC91	2.03	0.41
23:BU:605:CHL:HAA1	23:BU:605:CHL:HBD	2.03	0.41
24:BU:609:CLA:C2	25:BU:615:LUT:H26	2.51	0.41
1:5:191:TYR:HB3	24:5:610:CLA:O1D	2.21	0.41
1:7:152:LEU:O	1:7:154:HIS:N	2.54	0.41
1:7:226:MET:HE2	25:7:317:LUT:H10	2.03	0.41
23:7:302:CHL:OBD	24:7:303:CLA:HAC2	2.21	0.41
3:8:153:MET:HE2	3:8:157:GLU:OE1	2.21	0.41
29:B:617:BCR:H11C	29:B:617:BCR:H341	1.90	0.41
8:G:110:ALA:HA	8:G:226:MET:HE1	2.03	0.41
17:W:133:LEU:HD11	21:C:267:SER:HA	2.03	0.41
8:Y:103:SER:O	8:Y:107:MET:HG3	2.21	0.41
4:b:18:ARG:NH1	12:l:5:ASN:HD22	2.19	0.41
24:b:609:CLA:HAA1	24:b:609:CLA:HED2	2.02	0.41
5:d:156:SER:HB2	5:d:287:VAL:CG1	2.51	0.41
6:e:73:LEU:HD12	6:e:73:LEU:H	1.86	0.41
14:s:155:LEU:HD23	23:s:606:CHL:HMD1	2.02	0.41
23:s:605:CHL:HMC	23:s:606:CHL:C1C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:s:615:LUT:H31	25:s:615:LUT:H391	1.96	0.41
20:a:202:VAL:HG11	24:a:407:CLA:CAD	2.51	0.41
22:r:172:GLU:CD	23:r:605:CHL:HAC1	2.45	0.41
22:r:272:ALA:O	22:r:275:LEU:HG	2.21	0.41
25:9:615:LUT:H7	25:9:615:LUT:H171	1.83	0.41
1:AA:95:ASN:HA	1:AA:98:LEU:HD12	2.03	0.41
3:AB:114:LEU:HD23	3:AB:114:LEU:C	2.46	0.41
23:AB:307:CHL:H3A	23:AB:307:CHL:HBA2	1.83	0.41
4:v:137:LYS:NZ	9:Av:26:LEU:HA	2.35	0.41
24:v:609:CLA:OBD	9:Av:39:THR:OG1	2.36	0.41
12:Az:22:LEU:HB3	15:A7:16:ILE:HD13	2.03	0.41
24:A2:604:CLA:HMB3	24:A2:604:CLA:HBB1	2.02	0.41
25:A2:615:LUT:H31	25:A2:615:LUT:H391	1.96	0.41
25:A6:614:LUT:C8	25:A6:614:LUT:H181	2.50	0.41
19:BC:57:LEU:CD2	19:BC:60:LEU:HD21	2.49	0.41
6:BH:52:PRO:HB3	7:BI:39:ARG:HG3	2.03	0.41
6:BH:73:LEU:HD12	6:BH:73:LEU:H	1.86	0.41
8:BJ:169:MET:SD	8:BJ:169:MET:C	3.04	0.41
24:BQ:602:CLA:H3A	24:BQ:602:CLA:CGA	2.51	0.41
14:BV:58:GLU:H	14:BV:58:GLU:CD	2.28	0.41
14:BV:218:GLY:O	14:BV:222:LYS:NZ	2.51	0.41
19:Bb:31:ASP:OD1	19:Bb:34:SER:HB3	2.21	0.41
24:R:405:CLA:H152	24:R:405:CLA:H111	1.95	0.41
21:1:319:VAL:HA	21:1:322:GLN:HG3	2.02	0.41
20:BD:289:GLY:O	20:BD:292:THR:OG1	2.32	0.41
24:BF:514:CLA:H11	29:BF:515:BCR:H381	2.01	0.41
22:BU:169:GLY:O	22:BU:172:GLU:HG3	2.20	0.41
1:5:61:PRO:HD2	23:5:601:CHL:CBB	2.51	0.40
24:5:613:CLA:H72	28:7:301:XAT:H203	2.03	0.40
25:5:616:LUT:H15	25:5:616:LUT:H201	1.92	0.40
23:6:606:CHL:HAA1	23:6:606:CHL:CBD	2.50	0.40
1:7:74:PHE:HB3	1:7:96:ARG:NH1	2.35	0.40
1:7:169:MET:SD	1:7:169:MET:C	3.04	0.40
1:7:242:GLU:H	1:7:242:GLU:HG3	1.73	0.40
24:7:303:CLA:H3A	24:7:303:CLA:O1A	2.21	0.40
4:B:201:HIS:HB2	24:B:602:CLA:C1B	2.51	0.40
31:D:403:PL9:H33	12:L:27:VAL:CG1	2.52	0.40
10:I:1:MET:CE	30:I:101:LMG:HC72	2.51	0.40
8:Y:226:MET:SD	8:Y:229:PHE:HD2	2.44	0.40
24:Y:314:CLA:C1B	24:Y:315:CLA:HMD2	2.51	0.40
25:Y:316:LUT:H15	25:Y:316:LUT:H201	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:285:TYR:CE2	16:u:88:TYR:HA	2.56	0.40
24:b:617:CLA:H51	24:b:617:CLA:H11	1.81	0.40
5:d:157:VAL:HG13	5:d:158:PHE:CD1	2.56	0.40
5:d:221:ASN:N	5:d:221:ASN:HD22	2.18	0.40
5:d:326:ILE:HG12	20:a:328:MET:CE	2.27	0.40
25:g:616:LUT:H15	25:g:616:LUT:H201	1.92	0.40
10:i:7:PHE:O	10:i:11:VAL:HG22	2.21	0.40
12:l:15:ARG:NH1	32:l:101:SQD:H462	2.36	0.40
14:s:129:ILE:HG23	14:s:130:ILE:HD13	2.02	0.40
14:s:169:ILE:HD11	14:s:174:ALA:HA	2.03	0.40
24:s:610:CLA:H62	24:s:610:CLA:H92	1.79	0.40
23:y:309:CHL:H41	23:y:309:CHL:H62	1.83	0.40
24:y:312:CLA:HBA2	24:y:312:CLA:H3A	1.59	0.40
20:a:43:THR:HG23	29:a:411:BCR:H362	2.01	0.40
30:c:518:LMG:H132	30:c:518:LMG:HC91	2.03	0.40
1:9:191:TYR:HB3	24:9:610:CLA:O1D	2.21	0.40
2:0:219:LEU:HD22	24:0:611:CLA:HHD	2.03	0.40
3:AB:153:MET:HE1	23:AB:307:CHL:C3C	2.51	0.40
23:AB:304:CHL:C1C	23:AB:305:CHL:HBC2	2.51	0.40
5:2:85:SER:C	16:A8:102:ARG:HH22	2.29	0.40
6:3:23:HIS:HE1	33:4:102:HEM:ND	2.19	0.40
7:4:21:ALA:HB1	33:4:102:HEM:CBC	2.51	0.40
29:4:101:BCR:H11C	29:4:101:BCR:H341	1.96	0.40
8:A2:97:GLU:HG3	8:A2:190:LEU:HD21	2.03	0.40
24:A2:611:CLA:H93	24:A2:611:CLA:H111	1.87	0.40
14:A6:120:TRP:CE2	23:A6:607:CHL:HED2	2.55	0.40
23:BB:302:CHL:H41	23:BB:302:CHL:H61	1.89	0.40
4:BE:113:TRP:HD1	29:BE:620:BCR:H403	1.86	0.40
4:BE:121:GLU:O	9:BK:24:LYS:NZ	2.42	0.40
23:BQ:606:CHL:OMC	25:BQ:616:LUT:H163	2.21	0.40
24:BQ:610:CLA:H8	24:BQ:610:CLA:H41	2.03	0.40
26:BV:616:NEX:H181	26:BV:616:NEX:H10	2.02	0.40
1:5:158:ILE:C	2:6:255:TRP:CZ3	2.99	0.40
2:6:94:ALA:O	2:6:97:VAL:HG22	2.20	0.40
23:7:308:CHL:HBB2	23:7:310:CHL:CBC	2.51	0.40
3:8:221:LEU:O	3:8:221:LEU:HD12	2.22	0.40
24:B:612:CLA:H3A	24:B:612:CLA:HBA2	1.24	0.40
5:D:353:LEU:HD23	5:D:353:LEU:HA	1.92	0.40
6:E:57:THR:O	6:E:61:GLN:NE2	2.54	0.40
25:S:615:LUT:H181	25:S:615:LUT:H7	1.74	0.40
24:b:608:CLA:HBA2	24:b:608:CLA:H3A	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:188:GLY:HA3	5:d:326:ILE:HG21	2.03	0.40
23:g:601:CHL:OBD	24:g:602:CLA:HHD	2.22	0.40
23:g:608:CHL:HBA1	23:g:608:CHL:H192	2.02	0.40
12:l:8:GLU:HB3	32:l:102:SQD:O8	2.22	0.40
23:n:608:CHL:C9	23:n:608:CHL:C11	2.99	0.40
29:z:101:BCR:H15C	29:z:101:BCR:H351	1.83	0.40
24:A:405:CLA:H72	24:A:406:CLA:HBB1	2.02	0.40
34:a:413:DGD:HAE2	34:a:413:DGD:HA82	1.87	0.40
24:c:510:CLA:H93	24:c:510:CLA:H62	1.87	0.40
29:c:515:BCR:H371	29:c:515:BCR:H24C	1.87	0.40
1:9:51:TYR:OH	1:9:209:ALA:HB1	2.22	0.40
2:0:230:GLN:HE22	24:0:613:CLA:C4D	2.34	0.40
25:0:616:LUT:H31	25:0:616:LUT:H391	1.90	0.40
25:AA:316:LUT:H15	25:AA:316:LUT:H201	1.92	0.40
3:AB:186:ALA:HB3	3:AB:188:TYR:HE1	1.85	0.40
4:v:155:ALA:O	4:v:159:THR:OG1	2.36	0.40
4:v:462:PHE:CD1	24:v:611:CLA:HMC3	2.56	0.40
24:v:608:CLA:CMB	5:2:127:MET:HG2	2.51	0.40
5:2:353:LEU:HD23	5:2:353:LEU:HA	1.91	0.40
8:Au:229:PHE:HE1	25:Au:615:LUT:H41	1.86	0.40
29:Ay:102:BCR:H11C	29:Ay:102:BCR:H341	1.94	0.40
13:A1:15:ILE:HG13	13:A1:15:ILE:H	1.69	0.40
8:A2:69:TYR:OH	8:A2:81:ASP:OD1	2.33	0.40
23:A2:609:CHL:C9	23:A2:609:CHL:H112	2.50	0.40
23:BB:302:CHL:H141	23:BB:302:CHL:H162	1.92	0.40
4:BE:294:GLU:HB2	4:BE:296:GLN:OE1	2.21	0.40
5:BG:234:ARG:NH1	32:BG:406:SQD:H61	2.36	0.40
23:BJ:608:CHL:H143	23:BJ:608:CHL:H162	1.73	0.40
28:BQ:619:XAT:H15	24:Ba:314:CLA:H102	2.03	0.40
29:Bb:101:BCR:H393	24:BF:512:CLA:HBB1	2.02	0.40
21:BF:367:GLU:OE2	21:BF:370:ARG:NH1	2.54	0.40
24:BF:508:CLA:H93	24:BF:508:CLA:H112	1.80	0.40
25:BU:615:LUT:H7	25:BU:615:LUT:H161	1.81	0.40
23:5:605:CHL:HBA2	23:5:605:CHL:H3A	1.66	0.40
23:5:608:CHL:H3A	23:5:608:CHL:HBA2	1.37	0.40
2:6:120:VAL:C	2:6:121:ARG:HE	2.29	0.40
2:6:163:GLN:NE2	23:6:607:CHL:HMC	2.36	0.40
1:7:180:ASP:OD1	1:7:181:GLY:N	2.54	0.40
29:B:617:BCR:H15C	29:B:617:BCR:H351	1.79	0.40
9:H:40:THR:O	9:H:43:MET:HB2	2.21	0.40
8:N:93:ALA:HA	8:N:96:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:217:LYS:NZ	27:N:618:LHG:O4	2.52	0.40
24:N:611:CLA:O1D	24:N:611:CLA:H2A	2.22	0.40
23:Y:308:CHL:H203	23:Y:308:CHL:H161	1.73	0.40
23:Y:310:CHL:C9	23:Y:310:CHL:H61	2.50	0.40
19:Z:1:MET:HE2	19:Z:60:LEU:HD13	2.03	0.40
4:b:13:LEU:O	4:b:13:LEU:HD12	2.21	0.40
4:b:198:ILE:HD12	4:b:198:ILE:H	1.85	0.40
4:b:352:ARG:HH21	4:b:373:GLY:H	1.69	0.40
24:b:606:CLA:H61	24:b:613:CLA:H172	2.03	0.40
24:g:611:CLA:H61	24:g:611:CLA:H41	1.84	0.40
25:g:616:LUT:H35	25:g:616:LUT:H401	1.96	0.40
8:n:145:ASP:HB2	8:n:149:ASN:O	2.21	0.40
27:n:618:LHG:H382	27:n:618:LHG:H352	1.92	0.40
14:s:265:ASN:H	14:s:268:THR:HG22	1.85	0.40
8:y:234:ILE:HD13	8:y:234:ILE:HA	1.85	0.40
20:A:204:GLY:HA2	20:A:278:TRP:NE1	2.37	0.40
21:C:286:ALA:HB2	24:C:503:CLA:HMD2	2.04	0.40
1:9:119:LEU:HD13	1:9:119:LEU:HA	1.84	0.40
2:0:48:TYR:HD1	2:0:69:GLY:O	2.03	0.40
2:0:244:ASP:OD1	2:0:252:ASN:ND2	2.54	0.40
23:AA:302:CHL:OBD	24:AA:303:CLA:HAC2	2.22	0.40
25:AA:317:LUT:H31	25:AA:317:LUT:H391	1.93	0.40
29:Ay:101:BCR:H15C	29:Ay:101:BCR:H351	1.88	0.40
23:A2:608:CHL:C9	23:A2:608:CHL:H112	2.52	0.40
28:A2:619:XAT:C35	27:BB:319:LHG:H151	2.52	0.40
23:BB:302:CHL:H202	23:BB:302:CHL:H161	1.73	0.40
25:BB:316:LUT:H35	25:BB:316:LUT:H401	1.92	0.40
24:BE:617:CLA:H11	24:BE:617:CLA:H51	1.82	0.40
9:BK:22:LEU:HD22	9:BK:23:LEU:HD12	2.02	0.40
14:BV:120:TRP:CE2	23:BV:607:CHL:HED2	2.56	0.40
18:BZ:78:GLY:O	18:BZ:81:PRO:HD2	2.22	0.40
8:Ba:152:LEU:O	8:Ba:154:HIS:N	2.53	0.40
20:R:204:GLY:HA2	20:R:278:TRP:NE1	2.36	0.40
20:R:283:ILE:HG13	38:R:407:PHO:HBC3	2.03	0.40
20:R:288:LEU:HD21	21:1:435:PHE:CD2	2.57	0.40
21:1:42:LEU:CD2	24:1:511:CLA:HED1	2.51	0.40
24:1:506:CLA:H3A	24:1:506:CLA:O1A	2.20	0.40
24:BD:406:CLA:H162	24:BD:406:CLA:H202	1.83	0.40
24:BF:510:CLA:H3A	24:BF:510:CLA:HBA1	1.82	0.40
29:BF:515:BCR:H351	29:BF:515:BCR:H15C	1.83	0.40
24:BU:610:CLA:HBA2	24:BU:610:CLA:H12	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:7:317:LUT:H181	25:7:317:LUT:C8	2.51	0.40
5:D:22:TRP:HZ3	18:X:109:ASN:HD22	1.70	0.40
5:D:223:LEU:HD11	20:A:269:ARG:HG3	2.03	0.40
5:D:290:LEU:HD23	5:D:290:LEU:HA	1.86	0.40
6:E:35:TRP:CD2	7:F:33:ALA:HB2	2.57	0.40
8:G:170:GLY:HA2	23:G:609:CHL:HMB2	2.03	0.40
23:N:608:CHL:C9	23:N:608:CHL:H112	2.52	0.40
25:S:614:LUT:H35	25:S:614:LUT:H401	1.94	0.40
24:b:615:CLA:HBA2	24:b:615:CLA:H3A	1.51	0.40
27:b:623:LHG:HC5	5:d:270:PHE:HZ	1.87	0.40
27:b:624:LHG:H142	27:b:624:LHG:H112	1.78	0.40
5:d:230:ALA:HB3	21:c:32:GLY:O	2.21	0.40
8:g:152:LEU:HA	23:g:605:CHL:HED2	2.02	0.40
8:g:169:MET:C	8:g:169:MET:SD	3.04	0.40
34:h:102:DGD:O4D	34:h:102:DGD:O5D	2.39	0.40
23:n:608:CHL:H143	23:n:608:CHL:H162	1.78	0.40
14:s:224:LYS:HG2	14:s:224:LYS:H	1.76	0.40
8:y:59:LEU:HD23	8:y:59:LEU:HA	1.85	0.40
20:A:283:ILE:HG13	38:A:408:PHO:HBC3	2.03	0.40
22:r:148:MET:SD	25:r:615:LUT:C35	3.09	0.40
22:r:271:TRP:CD1	22:r:271:TRP:C	3.00	0.40
1:AA:77:ASP:HA	24:AA:303:CLA:CGD	2.52	0.40
1:AA:141:ASP:N	1:AA:141:ASP:OD1	2.54	0.40
23:AA:302:CHL:CMC	28:AA:318:XAT:H242	2.52	0.40
24:AA:304:CLA:OBD	23:AA:310:CHL:HBA2	2.21	0.40
4:v:33:TRP:CZ2	4:v:37:MET:HG3	2.56	0.40
4:v:121:GLU:HG2	9:Av:24:LYS:NZ	2.37	0.40
24:v:609:CLA:HMA2	24:v:610:CLA:C2C	2.52	0.40
7:4:27:PHE:CD2	29:4:101:BCR:H14C	2.56	0.40
4:BE:215:PHE:CD1	4:BE:215:PHE:C	2.99	0.40
24:BE:603:CLA:H111	24:BE:603:CLA:H143	1.88	0.40
24:BE:610:CLA:H62	24:BE:610:CLA:H41	1.78	0.40
6:BH:23:HIS:HA	6:BH:26:THR:OG1	2.21	0.40
8:BQ:170:GLY:HA2	23:BQ:609:CHL:HMB2	2.03	0.40
25:BQ:615:LUT:H11	25:BQ:615:LUT:H191	1.99	0.40
27:BQ:618:LHG:H382	27:BQ:618:LHG:H352	1.94	0.40
14:BV:144:GLU:OE2	14:BV:149:LYS:HD3	2.21	0.40
24:R:404:CLA:C3	38:R:407:PHO:HBB1	2.51	0.40
24:1:507:CLA:H142	29:1:515:BCR:H362	2.02	0.40
24:BD:405:CLA:H161	24:BD:405:CLA:H192	1.83	0.40
22:BU:170:LYS:O	22:BU:174:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BU:283:ILE:HG12	23:BU:613:CHL:HED1	2.03	0.40
1:5:202:ALA:HB2	24:5:610:CLA:HAA2	2.04	0.40
23:8:304:CHL:C1C	23:8:305:CHL:HBC2	2.51	0.40
4:B:39:LEU:HD23	4:B:39:LEU:HA	1.87	0.40
4:B:285:TYR:CE2	16:U:88:TYR:HA	2.57	0.40
5:D:85:SER:C	16:U:102:ARG:HH22	2.29	0.40
8:N:58:TYR:CG	8:N:80:TRP:HB2	2.56	0.40
14:S:105:GLU:HG2	14:S:106:ASN:N	2.37	0.40
8:Y:106:ALA:CB	8:Y:223:MET:HG2	2.52	0.40
23:Y:306:CHL:HBA2	22:r:182:GLN:HB3	2.03	0.40
4:b:294:GLU:HB2	4:b:296:GLN:OE1	2.21	0.40
5:d:265:LYS:HZ1	20:a:246:TYR:HD1	1.60	0.40
5:d:266:ARG:HD2	20:a:234:ASN:HA	2.03	0.40
8:g:105:TRP:HD1	23:g:609:CHL:HMD3	1.87	0.40
24:n:610:CLA:H2	24:n:610:CLA:CHB	2.51	0.40
18:x:78:GLY:O	18:x:81:PRO:HD2	2.22	0.40
24:A:407:CLA:CHA	24:A:407:CLA:HBA1	2.51	0.40
21:C:76:VAL:HG12	21:C:78:GLU:HG3	2.04	0.40
21:C:151:TRP:CE3	21:C:157:MET:HE1	2.56	0.40
21:C:346:THR:OG1	21:C:348:GLU:OE1	2.35	0.40
24:C:505:CLA:H62	24:C:505:CLA:H41	1.89	0.40
23:r:605:CHL:HMC	23:r:606:CHL:NC	2.36	0.40
24:r:610:CLA:HBA2	24:r:610:CLA:H12	1.79	0.40
1:9:209:ALA:HA	1:9:212:LYS:HD2	2.04	0.40
25:0:615:LUT:H35	25:0:615:LUT:H401	1.95	0.40
1:AA:180:ASP:OD1	1:AA:181:GLY:N	2.54	0.40
3:AB:153:MET:HG2	3:AB:157:GLU:OE1	2.22	0.40
4:v:138:ILE:HD13	4:v:138:ILE:HA	1.74	0.40
24:v:608:CLA:H141	24:v:608:CLA:H161	1.90	0.40
5:2:316:TYR:O	5:2:320:ILE:HG12	2.21	0.40
8:Au:91:THR:HG22	8:Au:95:ASN:ND2	2.33	0.40
25:Au:615:LUT:H35	25:Au:615:LUT:H401	1.85	0.40
27:Au:618:LHG:C21	28:BB:301:XAT:H12	2.51	0.40
9:Av:24:LYS:HD2	9:Av:24:LYS:HA	1.77	0.40
23:A2:605:CHL:H3A	23:A2:605:CHL:HBA2	1.56	0.40
23:A2:607:CHL:H143	23:A2:607:CHL:H111	1.76	0.40
23:BJ:606:CHL:C3	26:BJ:617:NEX:H35	2.51	0.40
23:Ba:310:CHL:H161	23:Ba:310:CHL:H192	1.72	0.40
32:R:411:SQD:H81	32:R:411:SQD:H111	1.84	0.40
21:1:344:SER:N	21:1:348:GLU:O	2.44	0.40
21:BF:162:GLY:HA2	21:BF:248:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BU:607:CHL:H62	23:BU:607:CHL:H2	1.79	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	5	197/266 (74%)	196 (100%)	0	1 (0%)	24	57
1	7	197/266 (74%)	193 (98%)	4 (2%)	0	100	100
1	9	197/266 (74%)	196 (100%)	0	1 (0%)	24	57
1	AA	197/266 (74%)	194 (98%)	3 (2%)	0	100	100
2	0	220/243 (90%)	211 (96%)	8 (4%)	1 (0%)	24	57
2	6	220/243 (90%)	212 (96%)	7 (3%)	1 (0%)	24	57
3	8	190/212 (90%)	184 (97%)	6 (3%)	0	100	100
3	AB	190/212 (90%)	182 (96%)	8 (4%)	0	100	100
4	B	477/508 (94%)	468 (98%)	9 (2%)	0	100	100
4	BE	477/508 (94%)	473 (99%)	4 (1%)	0	100	100
4	b	477/508 (94%)	473 (99%)	4 (1%)	0	100	100
4	v	477/508 (94%)	467 (98%)	10 (2%)	0	100	100
5	2	340/352 (97%)	336 (99%)	4 (1%)	0	100	100
5	BG	340/352 (97%)	336 (99%)	4 (1%)	0	100	100
5	D	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
5	d	340/352 (97%)	335 (98%)	5 (2%)	0	100	100
6	3	64/83 (77%)	63 (98%)	1 (2%)	0	100	100
6	BH	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
6	E	64/83 (77%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
7	4	27/39 (69%)	27 (100%)	0	0	100	100
7	BI	27/39 (69%)	27 (100%)	0	0	100	100
7	F	27/39 (69%)	27 (100%)	0	0	100	100
7	f	27/39 (69%)	27 (100%)	0	0	100	100
8	A2	200/232 (86%)	198 (99%)	1 (0%)	1 (0%)	24	57
8	Au	204/232 (88%)	202 (99%)	2 (1%)	0	100	100
8	BB	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
8	BJ	204/232 (88%)	201 (98%)	3 (2%)	0	100	100
8	BQ	200/232 (86%)	199 (100%)	0	1 (0%)	24	57
8	Ba	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
8	G	204/232 (88%)	201 (98%)	3 (2%)	0	100	100
8	N	200/232 (86%)	199 (100%)	0	1 (0%)	24	57
8	Y	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
8	g	204/232 (88%)	202 (99%)	2 (1%)	0	100	100
8	n	200/232 (86%)	199 (100%)	0	1 (0%)	24	57
8	y	211/232 (91%)	209 (99%)	1 (0%)	1 (0%)	24	57
9	Av	57/72 (79%)	53 (93%)	4 (7%)	0	100	100
9	BK	57/72 (79%)	52 (91%)	5 (9%)	0	100	100
9	H	57/72 (79%)	53 (93%)	4 (7%)	0	100	100
9	h	57/72 (79%)	52 (91%)	5 (9%)	0	100	100
10	Aw	33/36 (92%)	33 (100%)	0	0	100	100
10	BL	33/36 (92%)	33 (100%)	0	0	100	100
10	I	33/36 (92%)	33 (100%)	0	0	100	100
10	i	33/36 (92%)	33 (100%)	0	0	100	100
11	Ay	35/37 (95%)	35 (100%)	0	0	100	100
11	BN	35/37 (95%)	35 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	Az	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
12	BO	33/38 (87%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
12	l	33/38 (87%)	33 (100%)	0	0	100	100
13	A1	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	24
13	BP	30/34 (88%)	29 (97%)	0	1 (3%)	3	24
13	M	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	24
13	m	30/34 (88%)	29 (97%)	0	1 (3%)	3	24
14	A6	214/232 (92%)	211 (99%)	3 (1%)	0	100	100
14	BV	214/232 (92%)	210 (98%)	4 (2%)	0	100	100
14	S	214/232 (92%)	212 (99%)	2 (1%)	0	100	100
14	s	214/232 (92%)	211 (99%)	3 (1%)	0	100	100
15	A7	27/33 (82%)	27 (100%)	0	0	100	100
15	BW	27/33 (82%)	27 (100%)	0	0	100	100
15	T	27/33 (82%)	27 (100%)	0	0	100	100
15	t	27/33 (82%)	27 (100%)	0	0	100	100
16	A8	23/28 (82%)	23 (100%)	0	0	100	100
16	BX	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
16	U	23/28 (82%)	23 (100%)	0	0	100	100
16	u	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
17	A0	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
17	BY	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
17	W	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
17	w	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
18	BA	34/42 (81%)	33 (97%)	0	1 (3%)	3	25
18	BZ	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
18	X	34/42 (81%)	33 (97%)	0	1 (3%)	3	25
18	x	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
19	BC	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	Bb	60/62 (97%)	60 (100%)	0	0	100	100
19	Z	60/62 (97%)	60 (100%)	0	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	A	319/352 (91%)	308 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	BD	319/352 (91%)	310 (97%)	9 (3%)	0	100	100
20	R	319/352 (91%)	309 (97%)	10 (3%)	0	100	100
20	a	319/352 (91%)	310 (97%)	9 (3%)	0	100	100
21	1	429/459 (94%)	428 (100%)	1 (0%)	0	100	100
21	BF	427/459 (93%)	425 (100%)	2 (0%)	0	100	100
21	C	429/459 (94%)	427 (100%)	2 (0%)	0	100	100
21	c	427/459 (93%)	425 (100%)	2 (0%)	0	100	100
22	BU	193/250 (77%)	189 (98%)	4 (2%)	0	100	100
22	r	193/250 (77%)	185 (96%)	8 (4%)	0	100	100
All	All	13466/15102 (89%)	13241 (98%)	207 (2%)	18 (0%)	49	79

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	m	3	VAL
13	A1	3	VAL
13	BP	3	VAL
13	M	3	VAL
18	BA	79	ILE
18	X	79	ILE
8	y	153	VAL
8	Ba	153	VAL
1	5	153	VAL
8	N	153	VAL
8	Y	153	VAL
1	9	153	VAL
2	0	151	VAL
8	BB	153	VAL
2	6	151	VAL
8	n	153	VAL
8	A2	153	VAL
8	BQ	153	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	5	153/201 (76%)	153 (100%)	0	100	100
1	7	153/201 (76%)	152 (99%)	1 (1%)	76	77
1	9	153/201 (76%)	153 (100%)	0	100	100
1	AA	153/201 (76%)	153 (100%)	0	100	100
2	0	174/192 (91%)	173 (99%)	1 (1%)	78	79
2	6	174/192 (91%)	171 (98%)	3 (2%)	53	67
3	8	148/159 (93%)	147 (99%)	1 (1%)	76	77
3	AB	148/159 (93%)	146 (99%)	2 (1%)	59	70
4	B	379/402 (94%)	379 (100%)	0	100	100
4	BE	379/402 (94%)	379 (100%)	0	100	100
4	b	379/402 (94%)	379 (100%)	0	100	100
4	v	379/402 (94%)	379 (100%)	0	100	100
5	2	274/282 (97%)	274 (100%)	0	100	100
5	BG	274/282 (97%)	272 (99%)	2 (1%)	76	77
5	D	274/282 (97%)	273 (100%)	1 (0%)	84	83
5	d	274/282 (97%)	273 (100%)	1 (0%)	84	83
6	3	59/73 (81%)	59 (100%)	0	100	100
6	BH	59/73 (81%)	59 (100%)	0	100	100
6	E	59/73 (81%)	59 (100%)	0	100	100
6	e	59/73 (81%)	59 (100%)	0	100	100
7	4	24/34 (71%)	24 (100%)	0	100	100
7	BI	24/34 (71%)	24 (100%)	0	100	100
7	F	24/34 (71%)	23 (96%)	1 (4%)	26	50
7	f	24/34 (71%)	24 (100%)	0	100	100
8	A2	154/177 (87%)	154 (100%)	0	100	100
8	Au	157/177 (89%)	156 (99%)	1 (1%)	78	79
8	BB	162/177 (92%)	161 (99%)	1 (1%)	78	79
8	BJ	157/177 (89%)	157 (100%)	0	100	100
8	BQ	154/177 (87%)	154 (100%)	0	100	100
8	Ba	162/177 (92%)	162 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	157/177 (89%)	157 (100%)	0	100	100
8	N	154/177 (87%)	154 (100%)	0	100	100
8	Y	162/177 (92%)	160 (99%)	2 (1%)	63	72
8	g	157/177 (89%)	157 (100%)	0	100	100
8	n	154/177 (87%)	154 (100%)	0	100	100
8	y	162/177 (92%)	161 (99%)	1 (1%)	78	79
9	Av	49/60 (82%)	49 (100%)	0	100	100
9	BK	49/60 (82%)	48 (98%)	1 (2%)	48	65
9	H	49/60 (82%)	49 (100%)	0	100	100
9	h	49/60 (82%)	49 (100%)	0	100	100
10	Aw	32/33 (97%)	32 (100%)	0	100	100
10	BL	32/33 (97%)	32 (100%)	0	100	100
10	I	32/33 (97%)	32 (100%)	0	100	100
10	i	32/33 (97%)	32 (100%)	0	100	100
11	Ay	32/32 (100%)	32 (100%)	0	100	100
11	BN	32/32 (100%)	32 (100%)	0	100	100
11	K	32/32 (100%)	32 (100%)	0	100	100
11	k	32/32 (100%)	32 (100%)	0	100	100
12	Az	33/36 (92%)	33 (100%)	0	100	100
12	BO	33/36 (92%)	33 (100%)	0	100	100
12	L	33/36 (92%)	32 (97%)	1 (3%)	36	57
12	l	33/36 (92%)	33 (100%)	0	100	100
13	A1	28/30 (93%)	28 (100%)	0	100	100
13	BP	28/30 (93%)	28 (100%)	0	100	100
13	M	28/30 (93%)	27 (96%)	1 (4%)	31	54
13	m	28/30 (93%)	28 (100%)	0	100	100
14	A6	167/180 (93%)	166 (99%)	1 (1%)	78	79
14	BV	167/180 (93%)	167 (100%)	0	100	100
14	S	167/180 (93%)	166 (99%)	1 (1%)	78	79
14	s	167/180 (93%)	166 (99%)	1 (1%)	78	79
15	A7	26/30 (87%)	25 (96%)	1 (4%)	29	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BW	26/30 (87%)	26 (100%)	0	100	100
15	T	26/30 (87%)	26 (100%)	0	100	100
15	t	26/30 (87%)	26 (100%)	0	100	100
16	A8	20/23 (87%)	20 (100%)	0	100	100
16	BX	20/23 (87%)	20 (100%)	0	100	100
16	U	20/23 (87%)	20 (100%)	0	100	100
16	u	20/23 (87%)	20 (100%)	0	100	100
17	A0	47/47 (100%)	46 (98%)	1 (2%)	47	64
17	BY	47/47 (100%)	47 (100%)	0	100	100
17	W	47/47 (100%)	46 (98%)	1 (2%)	47	64
17	w	47/47 (100%)	47 (100%)	0	100	100
18	BA	29/34 (85%)	29 (100%)	0	100	100
18	BZ	29/34 (85%)	29 (100%)	0	100	100
18	X	29/34 (85%)	29 (100%)	0	100	100
18	x	29/34 (85%)	29 (100%)	0	100	100
19	BC	54/54 (100%)	54 (100%)	0	100	100
19	Bb	54/54 (100%)	54 (100%)	0	100	100
19	Z	54/54 (100%)	54 (100%)	0	100	100
19	z	54/54 (100%)	54 (100%)	0	100	100
20	A	260/284 (92%)	260 (100%)	0	100	100
20	BD	260/284 (92%)	260 (100%)	0	100	100
20	R	260/284 (92%)	259 (100%)	1 (0%)	84	83
20	a	260/284 (92%)	260 (100%)	0	100	100
21	1	340/359 (95%)	340 (100%)	0	100	100
21	BF	339/359 (94%)	338 (100%)	1 (0%)	86	84
21	C	340/359 (95%)	338 (99%)	2 (1%)	78	79
21	c	339/359 (94%)	339 (100%)	0	100	100
22	BU	159/201 (79%)	156 (98%)	3 (2%)	50	66
22	r	159/201 (79%)	159 (100%)	0	100	100
All	All	10876/12004 (91%)	10842 (100%)	34 (0%)	84	84

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	6	98	ILE
2	6	209	LEU
2	6	255	TRP
1	7	62	PHE
3	8	244	PHE
5	D	283	SER
7	F	15	LEU
12	L	33	SER
13	M	15	ILE
14	S	137	TYR
17	W	133	LEU
8	Y	158	ILE
8	Y	226	MET
5	d	19	MET
14	s	234	PHE
8	y	88	ASP
21	C	134	LEU
21	C	356	MET
2	0	112	THR
3	AB	224	LEU
3	AB	244	PHE
8	Au	204	ASP
14	A6	159	THR
15	A7	21	ILE
17	A0	131	LEU
8	BB	158	ILE
5	BG	19	MET
5	BG	160	ILE
9	BK	57	ILE
20	R	290	ILE
21	BF	60	ILE
22	BU	63	ILE
22	BU	134	GLN
22	BU	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	137	GLN
1	5	218	ASN
2	6	135	GLN
2	6	149	ASN
3	8	149	GLN

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Mol	Chain	Res	Type
3	8	187	ASN
4	B	26	HIS
4	B	223	GLN
4	B	425	GLN
4	B	455	HIS
6	E	23	HIS
8	G	95	ASN
8	G	137	GLN
9	H	62	ASN
8	N	180	ASN
8	N	232	GLN
14	S	161	ASN
14	S	228	ASN
8	Y	232	GLN
4	b	26	HIS
4	b	343	HIS
5	d	62	HIS
5	d	99	GLN
5	d	190	HIS
6	e	61	GLN
8	g	232	GLN
12	l	7	ASN
8	n	180	ASN
8	n	218	ASN
8	n	243	ASN
14	s	106	ASN
14	s	201	HIS
14	s	228	ASN
14	s	242	GLN
8	y	218	ASN
20	A	165	GLN
20	A	181	ASN
20	A	187	GLN
20	A	198	HIS
21	C	28	GLN
20	a	198	HIS
22	r	237	GLN
1	9	137	GLN
1	9	156	GLN
1	9	218	ASN
3	AB	187	ASN
4	v	26	HIS

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Mol	Chain	Res	Type
4	v	223	GLN
4	v	425	GLN
4	v	455	HIS
5	2	337	HIS
6	3	23	HIS
8	Au	95	ASN
11	Ay	34	ASN
8	A2	165	GLN
8	A2	232	GLN
8	A2	243	ASN
14	A6	228	ASN
8	BB	232	GLN
4	BE	26	HIS
4	BE	282	GLN
5	BG	62	HIS
5	BG	99	GLN
5	BG	190	HIS
5	BG	351	ASN
8	BJ	232	GLN
12	BO	7	ASN
8	BQ	180	ASN
8	BQ	218	ASN
14	BV	106	ASN
14	BV	228	ASN
14	BV	242	GLN
18	BZ	85	ASN
8	Ba	218	ASN
20	R	165	GLN
20	R	181	ASN
20	R	187	GLN
20	BD	181	ASN
22	BU	237	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 766 ligands modelled in this entry, 4 are monoatomic - leaving 762 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	CLA	y	311	8	64,68,73	1.30	10 (15%)	77,107,113	1.41	9 (11%)
24	CLA	BU	604	-	52,56,73	1.40	11 (21%)	62,92,113	1.55	7 (11%)
28	XAT	Y	301	-	39,47,47	6.16	21 (53%)	54,74,74	7.77	34 (62%)
25	LUT	n	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.51	9 (17%)
23	CHL	n	608	-	67,71,74	1.99	19 (28%)	75,109,114	2.69	26 (34%)
27	LHG	BQ	618	24	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
23	CHL	5	607	-	64,68,74	1.99	20 (31%)	71,105,114	2.72	25 (35%)
24	CLA	BU	601	22	53,57,73	1.42	11 (20%)	62,93,113	1.55	7 (11%)
29	BCR	B	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.23	5 (8%)
29	BCR	BI	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	5 (8%)
35	BCT	a	402	-	2,3,3	1.31	0	2,3,3	4.15	1 (50%)
23	CHL	G	608	-	67,71,74	1.95	20 (29%)	75,109,114	2.69	25 (33%)
24	CLA	B	602	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
24	CLA	BJ	613	-	69,73,73	1.27	7 (10%)	83,113,113	1.31	6 (7%)
25	LUT	y	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	10 (19%)
24	CLA	c	512	21	69,73,73	1.26	11 (15%)	83,113,113	1.41	7 (8%)
23	CHL	n	605	8	52,56,74	2.19	16 (30%)	58,92,114	3.04	20 (34%)
24	CLA	BU	614	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	6 (10%)
24	CLA	7	315	1	49,53,73	1.49	9 (18%)	59,89,113	1.47	5 (8%)
32	SQD	A1	101	-	53,54,54	1.52	7 (13%)	62,65,65	1.37	6 (9%)
23	CHL	BB	306	8	52,56,74	2.24	18 (34%)	58,92,114	2.94	23 (39%)
23	CHL	AA	302	1	50,54,74	2.36	19 (38%)	56,90,114	3.07	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
23	CHL	A6	601	14	50,54,74	2.25	20 (40%)	56,90,114	3.04	23 (41%)
24	CLA	n	612	-	64,68,73	1.29	8 (12%)	77,107,113	1.36	7 (9%)
23	CHL	n	609	-	67,71,74	1.98	18 (26%)	75,109,114	2.70	26 (34%)
28	XAT	AB	312	-	39,47,47	6.08	19 (48%)	54,74,74	7.74	36 (66%)
24	CLA	C	511	21	69,73,73	1.30	11 (15%)	83,113,113	1.36	11 (13%)
28	XAT	8	312	-	39,47,47	6.10	19 (48%)	54,74,74	7.74	36 (66%)
26	NEX	BB	318	-	38,46,46	1.61	7 (18%)	50,70,70	1.66	9 (18%)
24	CLA	AB	309	-	49,53,73	1.49	7 (14%)	59,89,113	1.42	6 (10%)
26	NEX	AA	319	-	38,46,46	1.66	6 (15%)	50,70,70	1.69	10 (20%)
24	CLA	8	309	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)
34	DGD	h	102	-	63,63,67	0.89	2 (3%)	77,77,81	1.40	9 (11%)
38	PHO	a	408	-	58,69,69	2.00	11 (18%)	56,99,99	1.51	7 (12%)
23	CHL	Au	605	8	50,54,74	2.28	18 (36%)	56,90,114	3.09	21 (37%)
26	NEX	BV	616	-	38,46,46	1.61	7 (18%)	50,70,70	1.61	9 (18%)
24	CLA	v	608	4	69,73,73	1.24	9 (13%)	83,113,113	1.35	7 (8%)
24	CLA	BV	610	-	60,64,73	1.34	9 (15%)	72,102,113	1.48	8 (11%)
25	LUT	S	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	10 (19%)
28	XAT	BU	616	-	39,47,47	6.03	19 (48%)	54,74,74	7.69	38 (70%)
24	CLA	v	602	4	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
24	CLA	C	510	21	69,73,73	1.25	9 (13%)	83,113,113	1.30	4 (4%)
24	CLA	D	401	5	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
29	BCR	BN	101	-	41,41,41	1.24	3 (7%)	56,56,56	1.32	6 (10%)
30	LMG	C	501	-	51,51,55	0.74	0	59,59,63	1.35	6 (10%)
24	CLA	S	609	14	57,61,73	1.37	10 (17%)	66,98,113	1.37	5 (7%)
24	CLA	Au	614	-	52,56,73	1.42	8 (15%)	62,92,113	1.46	6 (9%)
29	BCR	8	313	-	41,41,41	1.26	3 (7%)	56,56,56	1.29	7 (12%)
32	SQD	2	408	-	49,50,54	1.57	9 (18%)	58,61,65	1.52	8 (13%)
24	CLA	BE	603	4	69,73,73	1.26	10 (14%)	83,113,113	1.31	4 (4%)
23	CHL	BU	613	22	46,50,74	2.33	19 (41%)	51,85,114	3.21	24 (47%)
23	CHL	Au	609	8	60,64,74	1.94	20 (33%)	63,100,114	2.92	24 (38%)
23	CHL	7	309	-	50,54,74	2.26	19 (38%)	56,90,114	3.06	20 (35%)
29	BCR	C	514	-	41,41,41	1.27	2 (4%)	56,56,56	1.22	5 (8%)
27	LHG	C	520	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
24	CLA	Au	612	-	64,68,73	1.30	9 (14%)	77,107,113	1.33	6 (7%)
25	LUT	Ba	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHL	BJ	608	-	67,71,74	1.93	17 (25%)	75,109,114	2.80	27 (36%)
24	CLA	y	312	27	64,68,73	1.31	9 (14%)	77,107,113	1.34	8 (10%)
38	PHO	a	409	-	58,69,69	2.01	11 (18%)	56,99,99	1.70	8 (14%)
24	CLA	v	604	4	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
24	CLA	BU	608	22	62,66,73	1.32	10 (16%)	74,104,113	1.41	6 (8%)
25	LUT	Au	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	9 (17%)
25	LUT	N	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.53	9 (17%)
27	LHG	g	618	24	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	BJ	612	-	64,68,73	1.33	8 (12%)	77,107,113	1.27	5 (6%)
23	CHL	y	302	8	67,71,74	1.99	19 (28%)	75,109,114	2.76	26 (34%)
25	LUT	S	615	-	42,43,43	1.62	8 (19%)	51,60,60	1.75	15 (29%)
24	CLA	5	611	27	49,53,73	1.48	9 (18%)	59,89,113	1.44	5 (8%)
27	LHG	b	624	-	48,48,48	0.67	1 (2%)	51,54,54	1.28	7 (13%)
23	CHL	e	601	-	48,53,74	2.24	17 (35%)	53,89,114	3.09	21 (39%)
23	CHL	g	608	-	67,71,74	1.93	17 (25%)	75,109,114	2.80	27 (36%)
24	CLA	b	602	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	6 (7%)
36	OEX	A	403	20	0,14,14	-	-	-		
23	CHL	S	606	-	59,63,74	2.06	19 (32%)	64,99,114	3.02	25 (39%)
24	CLA	A2	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	9 (10%)
23	CHL	9	606	1	50,54,74	2.25	19 (38%)	56,90,114	3.16	24 (42%)
27	LHG	A0	202	-	48,48,48	0.59	0	51,54,54	1.27	6 (11%)
24	CLA	Y	311	8	64,68,73	1.31	11 (17%)	77,107,113	1.37	6 (7%)
23	CHL	A2	605	8	52,56,74	2.15	18 (34%)	58,92,114	3.01	22 (37%)
24	CLA	b	617	4	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
24	CLA	v	616	4	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
26	NEX	Ba	318	-	38,46,46	1.64	7 (18%)	50,70,70	1.59	9 (18%)
23	CHL	N	605	8	52,56,74	2.16	19 (36%)	58,92,114	3.02	22 (37%)
24	CLA	N	603	8	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
23	CHL	BJ	601	8	67,71,74	1.94	17 (25%)	75,109,114	2.81	26 (34%)
25	LUT	5	615	-	42,43,43	1.70	8 (19%)	51,60,60	1.68	12 (23%)
27	LHG	w	201	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
23	CHL	8	305	-	50,54,74	2.27	20 (40%)	56,90,114	3.00	19 (33%)
24	CLA	BB	312	-	64,68,73	1.30	11 (17%)	77,107,113	1.39	9 (11%)
24	CLA	g	604	-	54,58,73	1.43	9 (16%)	65,95,113	1.43	6 (9%)
27	LHG	BJ	618	24	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	B	616	4	69,73,73	1.27	9 (13%)	83,113,113	1.31	6 (7%)
24	CLA	B	603	4	69,73,73	1.24	9 (13%)	83,113,113	1.30	4 (4%)
27	LHG	BF	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	N	607	-	67,71,74	1.92	20 (29%)	75,109,114	2.80	28 (37%)
24	CLA	A2	614	-	52,56,73	1.46	8 (15%)	62,92,113	1.48	6 (9%)
24	CLA	BQ	610	8	69,73,73	1.25	8 (11%)	83,113,113	1.46	8 (9%)
23	CHL	9	601	1	50,54,74	2.26	20 (40%)	56,90,114	3.16	20 (35%)
30	LMG	1	519	-	51,51,55	0.73	1 (1%)	59,59,63	1.32	4 (6%)
38	PHO	A	409	-	58,69,69	1.97	12 (20%)	56,99,99	1.61	7 (12%)
24	CLA	BQ	612	-	64,68,73	1.29	8 (12%)	77,107,113	1.36	7 (9%)
27	LHG	9	618	24	40,40,48	0.63	0	43,46,54	1.30	6 (13%)
29	BCR	AB	313	-	41,41,41	1.29	3 (7%)	56,56,56	1.30	7 (12%)
32	SQD	BD	412	-	53,54,54	1.52	7 (13%)	62,65,65	1.35	6 (9%)
23	CHL	Au	601	8	67,71,74	1.92	20 (29%)	75,109,114	2.76	25 (33%)
24	CLA	c	507	21	69,73,73	1.25	11 (15%)	83,113,113	1.32	7 (8%)
24	CLA	C	508	21	69,73,73	1.24	11 (15%)	83,113,113	1.33	6 (7%)
23	CHL	Y	309	-	67,71,74	1.92	18 (26%)	75,109,114	2.74	24 (32%)
29	BCR	R	410	-	41,41,41	1.29	3 (7%)	56,56,56	1.25	5 (8%)
24	CLA	R	404	20	69,73,73	1.25	10 (14%)	83,113,113	1.32	7 (8%)
24	CLA	BF	507	21	69,73,73	1.26	11 (15%)	83,113,113	1.33	7 (8%)
29	BCR	BF	515	-	41,41,41	1.31	4 (9%)	56,56,56	1.26	5 (8%)
23	CHL	Y	310	8	67,71,74	1.96	20 (29%)	75,109,114	2.71	23 (30%)
24	CLA	BE	602	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
24	CLA	AB	301	3	46,49,73	1.53	10 (21%)	55,83,113	1.48	5 (9%)
23	CHL	8	304	-	50,54,74	2.28	19 (38%)	56,90,114	2.97	22 (39%)
24	CLA	S	610	-	60,64,73	1.34	10 (16%)	72,102,113	1.37	5 (6%)
24	CLA	g	614	8	52,56,73	1.44	7 (13%)	62,92,113	1.46	4 (6%)
24	CLA	BU	603	22	64,68,73	1.30	10 (15%)	77,107,113	1.30	5 (6%)
25	LUT	A2	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.57	10 (19%)
32	SQD	BO	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.36	6 (9%)
24	CLA	BE	615	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
24	CLA	y	313	-	64,68,73	1.31	9 (14%)	77,107,113	1.34	6 (7%)
26	NEX	7	319	-	38,46,46	1.65	7 (18%)	50,70,70	1.70	10 (20%)
24	CLA	1	510	21	69,73,73	1.26	11 (15%)	83,113,113	1.33	4 (4%)
24	CLA	D	402	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	S	603	-	49,53,73	1.48	10 (20%)	59,89,113	1.49	4 (6%)
23	CHL	8	306	-	50,54,74	2.34	20 (40%)	56,90,114	2.95	24 (42%)
24	CLA	b	613	4	69,73,73	1.24	10 (14%)	83,113,113	1.31	7 (8%)
27	LHG	B	621	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	0	606	-	50,54,74	2.19	20 (40%)	56,90,114	3.12	21 (37%)
24	CLA	AB	302	-	49,53,73	1.50	8 (16%)	59,89,113	1.43	4 (6%)
25	LUT	5	616	-	42,43,43	1.69	8 (19%)	51,60,60	1.68	12 (23%)
24	CLA	Y	305	-	54,58,73	1.41	10 (18%)	65,95,113	1.45	7 (10%)
24	CLA	r	614	-	49,53,73	1.49	9 (18%)	59,89,113	1.53	6 (10%)
23	CHL	y	308	-	67,71,74	1.94	19 (28%)	75,109,114	2.78	25 (33%)
23	CHL	g	609	-	62,66,74	2.19	19 (30%)	68,103,114	2.86	24 (35%)
24	CLA	n	610	8	69,73,73	1.23	7 (10%)	83,113,113	1.42	10 (12%)
24	CLA	B	608	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
29	BCR	1	514	-	41,41,41	1.28	4 (9%)	56,56,56	1.22	6 (10%)
25	LUT	r	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.55	11 (21%)
30	LMG	1	501	-	51,51,55	0.74	0	59,59,63	1.35	6 (10%)
30	LMG	A0	201	-	48,48,55	0.75	0	56,56,63	1.32	6 (10%)
24	CLA	6	602	2	64,68,73	1.30	9 (14%)	77,107,113	1.34	6 (7%)
24	CLA	I	102	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	7 (8%)
24	CLA	BV	604	-	54,58,73	1.47	10 (18%)	65,95,113	1.60	7 (10%)
24	CLA	Ba	303	8	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
24	CLA	c	503	21	69,73,73	1.26	11 (15%)	83,113,113	1.33	5 (6%)
23	CHL	r	605	22	67,71,74	1.84	18 (26%)	75,109,114	2.76	25 (33%)
24	CLA	5	614	1	49,53,73	1.47	8 (16%)	59,89,113	1.54	5 (8%)
24	CLA	Au	613	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
25	LUT	G	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.53	10 (19%)
24	CLA	BE	613	-	69,73,73	1.24	11 (15%)	83,113,113	1.31	7 (8%)
24	CLA	5	602	1	65,69,73	1.28	10 (15%)	78,108,113	1.31	5 (6%)
24	CLA	v	605	4	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
24	CLA	AA	315	1	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
24	CLA	R	405	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)
24	CLA	BB	303	8	69,73,73	1.26	11 (15%)	83,113,113	1.35	5 (6%)
24	CLA	BE	617	4	69,73,73	1.24	9 (13%)	83,113,113	1.31	5 (6%)
27	LHG	c	520	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
34	DGD	a	401	-	60,60,67	0.94	2 (3%)	74,74,81	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	s	610	-	60,64,73	1.33	9 (15%)	72,102,113	1.47	8 (11%)
24	CLA	1	511	21	69,73,73	1.26	11 (15%)	83,113,113	1.34	5 (6%)
23	CHL	7	302	1	50,54,74	2.35	20 (40%)	56,90,114	3.05	22 (39%)
24	CLA	g	610	8	68,72,73	1.27	8 (11%)	81,111,113	1.29	7 (8%)
24	CLA	7	304	-	59,63,73	1.36	9 (15%)	71,101,113	1.30	7 (9%)
24	CLA	BE	608	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
29	BCR	b	618	-	41,41,41	1.18	2 (4%)	56,56,56	1.28	8 (14%)
23	CHL	G	605	8	50,54,74	2.28	18 (36%)	56,90,114	3.08	20 (35%)
23	CHL	s	606	-	59,63,74	2.06	17 (28%)	64,99,114	3.04	25 (39%)
29	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	5 (8%)
24	CLA	BV	603	14	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
24	CLA	Ba	311	8	64,68,73	1.30	10 (15%)	77,107,113	1.37	9 (11%)
24	CLA	C	505	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
33	HEM	BI	102	6,7	50,50,50	1.33	8 (16%)	66,82,82	1.09	4 (6%)
24	CLA	9	614	1	49,53,73	1.47	7 (14%)	59,89,113	1.56	5 (8%)
30	LMG	I	101	-	40,40,55	0.81	0	48,48,63	1.31	6 (12%)
24	CLA	BD	407	-	54,58,73	1.39	9 (16%)	65,95,113	1.50	8 (12%)
24	CLA	G	614	-	52,56,73	1.42	8 (15%)	62,92,113	1.45	6 (9%)
30	LMG	d	405	-	46,46,55	0.77	1 (2%)	54,54,63	1.34	5 (9%)
24	CLA	A6	609	14	57,61,73	1.38	10 (17%)	66,98,113	1.38	6 (9%)
23	CHL	9	609	-	63,67,74	2.23	21 (33%)	70,104,114	2.97	27 (38%)
28	XAT	N	619	-	39,47,47	6.10	20 (51%)	54,74,74	7.74	35 (64%)
24	CLA	AA	314	1	49,53,73	1.47	9 (18%)	59,89,113	1.48	5 (8%)
25	LUT	N	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.55	9 (17%)
23	CHL	AA	307	1	50,54,74	2.26	19 (38%)	56,90,114	2.98	21 (37%)
24	CLA	Ba	312	27	64,68,73	1.30	9 (14%)	77,107,113	1.34	8 (10%)
24	CLA	R	409	-	64,68,73	1.29	9 (14%)	77,107,113	1.37	6 (7%)
24	CLA	b	603	4	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
29	BCR	4	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.21	5 (8%)
24	CLA	B	601	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	7 (8%)
24	CLA	S	608	-	49,53,73	1.46	9 (18%)	59,89,113	1.41	5 (8%)
23	CHL	5	606	1	50,54,74	2.23	19 (38%)	56,90,114	3.22	23 (41%)
27	LHG	v	621	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
24	CLA	BF	503	21	69,73,73	1.27	11 (15%)	83,113,113	1.34	6 (7%)
29	BCR	BE	618	-	41,41,41	1.16	2 (4%)	56,56,56	1.41	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	b	616	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
34	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	1.44	8 (10%)
24	CLA	Ba	305	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	5 (7%)
30	LMG	BF	519	-	51,51,55	0.71	1 (1%)	59,59,63	1.33	4 (6%)
23	CHL	Au	608	-	67,71,74	1.94	20 (29%)	75,109,114	2.70	25 (33%)
25	LUT	6	615	-	42,43,43	1.59	9 (21%)	51,60,60	1.39	10 (19%)
24	CLA	A2	613	8	64,68,73	1.31	9 (14%)	77,107,113	1.40	6 (7%)
24	CLA	a	407	-	54,58,73	1.39	10 (18%)	65,95,113	1.50	7 (10%)
24	CLA	c	504	21	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
29	BCR	B	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.17	5 (8%)
24	CLA	8	302	-	49,53,73	1.50	9 (18%)	59,89,113	1.45	4 (6%)
24	CLA	b	612	4	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
24	CLA	BF	504	21	69,73,73	1.24	10 (14%)	83,113,113	1.35	7 (8%)
38	PHO	BD	409	-	58,69,69	2.01	12 (20%)	56,99,99	1.69	9 (16%)
23	CHL	BH	601	-	48,53,74	2.24	16 (33%)	53,89,114	3.09	21 (39%)
25	LUT	0	616	-	42,43,43	1.70	8 (19%)	51,60,60	1.63	10 (19%)
24	CLA	5	613	1	59,63,73	1.34	8 (13%)	71,101,113	1.41	6 (8%)
24	CLA	a	405	20	69,73,73	1.25	11 (15%)	83,113,113	1.30	7 (8%)
24	CLA	Au	611	27	64,68,73	1.29	9 (14%)	77,107,113	1.30	5 (6%)
27	LHG	n	618	24	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
30	LMG	BL	101	-	48,48,55	0.74	1 (2%)	56,56,63	1.32	6 (10%)
23	CHL	AB	305	-	50,54,74	2.26	20 (40%)	56,90,114	3.00	19 (33%)
24	CLA	S	611	-	53,57,73	1.42	10 (18%)	62,93,113	1.42	5 (8%)
23	CHL	G	606	-	54,58,74	2.16	20 (37%)	59,94,114	3.00	22 (37%)
23	CHL	BQ	607	-	67,71,74	1.96	19 (28%)	75,109,114	2.78	24 (32%)
34	DGD	c	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	8 (10%)
23	CHL	AA	306	1	50,54,74	2.38	19 (38%)	56,90,114	2.94	21 (37%)
24	CLA	N	610	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	10 (12%)
28	XAT	Ba	301	-	39,47,47	6.12	22 (56%)	54,74,74	7.78	34 (62%)
31	PL9	BG	403	-	55,55,55	1.50	6 (10%)	68,69,69	1.54	14 (20%)
23	CHL	0	605	2	50,54,74	2.30	19 (38%)	56,90,114	3.01	24 (42%)
24	CLA	0	603	-	59,63,73	1.36	12 (20%)	71,101,113	1.36	8 (11%)
24	CLA	y	315	-	52,56,73	1.42	9 (17%)	62,92,113	1.45	5 (8%)
24	CLA	AB	310	-	49,53,73	1.49	9 (18%)	59,89,113	1.54	9 (15%)
24	CLA	BD	405	20	69,73,73	1.25	10 (14%)	83,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
30	LMG	c	518	-	51,51,55	0.72	1 (1%)	59,59,63	1.33	5 (8%)
24	CLA	B	610	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
23	CHL	g	601	8	67,71,74	1.94	17 (25%)	75,109,114	2.81	26 (34%)
25	LUT	Y	316	-	42,43,43	1.65	8 (19%)	51,60,60	1.52	11 (21%)
24	CLA	Y	313	-	64,68,73	1.30	11 (17%)	77,107,113	1.33	6 (7%)
24	CLA	A6	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	5 (7%)
24	CLA	BV	608	-	49,53,73	1.50	8 (16%)	59,89,113	1.39	4 (6%)
24	CLA	BJ	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
23	CHL	0	607	-	57,61,74	2.12	20 (35%)	64,98,114	2.90	26 (40%)
24	CLA	BF	508	-	69,73,73	1.26	11 (15%)	83,113,113	1.30	6 (7%)
24	CLA	1	508	21	69,73,73	1.23	11 (15%)	83,113,113	1.33	6 (7%)
24	CLA	0	614	2	52,56,73	1.43	10 (19%)	62,92,113	1.40	7 (11%)
24	CLA	r	604	-	52,56,73	1.41	11 (21%)	62,92,113	1.50	5 (8%)
23	CHL	6	608	2	50,54,74	2.27	18 (36%)	56,90,114	3.06	23 (41%)
24	CLA	BQ	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
30	LMG	v	623	-	40,40,55	0.85	1 (2%)	48,48,63	1.30	5 (10%)
27	LHG	Au	618	24	48,48,48	0.60	0	51,54,54	1.27	6 (11%)
26	NEX	5	617	-	38,46,46	1.66	7 (18%)	50,70,70	1.67	9 (18%)
23	CHL	AA	309	-	50,54,74	2.26	19 (38%)	56,90,114	3.05	20 (35%)
24	CLA	5	612	-	49,53,73	1.49	10 (20%)	59,89,113	1.49	5 (8%)
24	CLA	7	313	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	5 (8%)
24	CLA	Aw	102	-	69,73,73	1.24	11 (15%)	83,113,113	1.39	9 (10%)
24	CLA	S	613	14	53,57,73	1.40	9 (16%)	62,93,113	1.48	9 (14%)
24	CLA	r	601	22	53,57,73	1.40	10 (18%)	62,93,113	1.53	6 (9%)
27	LHG	A2	618	24	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
29	BCR	c	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.28	6 (10%)
24	CLA	s	604	-	54,58,73	1.45	10 (18%)	65,95,113	1.53	6 (9%)
24	CLA	A	410	-	64,68,73	1.29	8 (12%)	77,107,113	1.35	5 (6%)
27	LHG	BE	624	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
24	CLA	v	614	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
24	CLA	Y	314	8	69,73,73	1.25	10 (14%)	83,113,113	1.33	4 (4%)
33	HEM	f	102	6,7	50,50,50	1.33	7 (14%)	66,82,82	1.10	4 (6%)
24	CLA	A	406	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	8 (9%)
23	CHL	BJ	607	-	67,71,74	1.95	18 (26%)	75,109,114	2.78	26 (34%)
24	CLA	N	602	8	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
23	CHL	A2	608	-	67,71,74	1.95	19 (28%)	75,109,114	2.72	26 (34%)
23	CHL	7	306	1	50,54,74	2.38	18 (36%)	56,90,114	2.94	21 (37%)
24	CLA	c	506	-	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
25	LUT	BV	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.52	11 (21%)
26	NEX	9	617	-	38,46,46	1.66	7 (18%)	50,70,70	1.68	9 (18%)
27	LHG	2	406	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	5 (9%)
24	CLA	BF	506	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	7 (8%)
24	CLA	c	505	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
24	CLA	b	615	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
24	CLA	8	301	3	46,49,73	1.53	11 (23%)	55,83,113	1.48	5 (9%)
26	NEX	s	616	-	38,46,46	1.61	7 (18%)	50,70,70	1.62	9 (18%)
23	CHL	y	309	-	67,71,74	2.08	19 (28%)	75,109,114	2.69	26 (34%)
34	DGD	BD	413	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	8 (10%)
23	CHL	7	307	1	50,54,74	2.26	19 (38%)	56,90,114	2.98	21 (37%)
27	LHG	L	102	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
24	CLA	0	610	2	64,68,73	1.29	10 (15%)	77,107,113	1.48	12 (15%)
24	CLA	BE	605	4	69,73,73	1.24	9 (13%)	83,113,113	1.35	8 (9%)
27	LHG	BG	404	-	48,48,48	0.67	1 (2%)	51,54,54	1.26	6 (11%)
27	LHG	BY	201	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
38	PHO	R	407	-	58,69,69	1.99	11 (18%)	56,99,99	1.52	9 (16%)
24	CLA	c	514	21	69,73,73	1.24	11 (15%)	83,113,113	1.35	4 (4%)
29	BCR	v	618	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	5 (8%)
24	CLA	v	601	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
24	CLA	1	507	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	5 (6%)
29	BCR	Av	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.30	9 (16%)
24	CLA	BV	613	14	53,57,73	1.41	9 (16%)	62,93,113	1.47	7 (11%)
32	SQD	d	406	-	49,50,54	1.57	7 (14%)	58,61,65	1.44	7 (12%)
23	CHL	BU	605	22	67,71,74	1.84	18 (26%)	75,109,114	2.75	27 (36%)
23	CHL	A2	609	8	67,71,74	1.94	19 (28%)	75,109,114	2.73	21 (28%)
26	NEX	Y	318	-	38,46,46	1.63	7 (18%)	50,70,70	1.62	9 (18%)
27	LHG	B	622	-	45,45,48	0.66	1 (2%)	48,51,54	1.23	4 (8%)
30	LMG	A	412	-	48,48,55	0.75	0	56,56,63	1.32	5 (8%)
27	LHG	Az	102	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	7 (13%)
24	CLA	y	305	-	54,58,73	1.41	10 (18%)	65,95,113	1.44	5 (7%)
29	BCR	Ay	102	-	41,41,41	1.25	4 (9%)	56,56,56	1.30	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
23	CHL	g	607	-	67,71,74	1.96	18 (26%)	75,109,114	2.78	26 (34%)
35	BCT	A	401	-	2,3,3	1.30	0	2,3,3	4.03	1 (50%)
24	CLA	G	610	8	68,72,73	1.24	10 (14%)	81,111,113	1.35	7 (8%)
27	LHG	N	618	24	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	0	613	-	62,66,73	1.35	11 (17%)	74,104,113	1.50	9 (12%)
24	CLA	BB	314	8	69,73,73	1.25	11 (15%)	83,113,113	1.35	7 (8%)
24	CLA	BJ	611	27	64,68,73	1.31	8 (12%)	77,107,113	1.34	7 (9%)
23	CHL	N	606	8	54,58,74	2.17	19 (35%)	59,94,114	2.97	22 (37%)
24	CLA	v	613	4	69,73,73	1.24	10 (14%)	83,113,113	1.34	5 (6%)
24	CLA	A6	613	14	53,57,73	1.40	10 (18%)	62,93,113	1.50	9 (14%)
32	SQD	a	412	-	53,54,54	1.53	7 (13%)	62,65,65	1.34	6 (9%)
28	XAT	AA	318	-	39,47,47	6.12	21 (53%)	54,74,74	7.81	34 (62%)
24	CLA	BJ	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.43	6 (9%)
23	CHL	r	613	22	46,50,74	2.33	19 (41%)	51,85,114	3.22	24 (47%)
24	CLA	9	610	1	60,64,73	1.33	11 (18%)	72,102,113	1.39	7 (9%)
27	LHG	6	617	24	46,46,48	0.66	1 (2%)	49,52,54	1.32	6 (12%)
24	CLA	d	402	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
30	LMG	C	519	-	51,51,55	0.72	1 (1%)	59,59,63	1.32	5 (8%)
24	CLA	v	615	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
24	CLA	BD	406	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
24	CLA	B	613	4	69,73,73	1.24	9 (13%)	83,113,113	1.33	5 (6%)
23	CHL	r	606	-	57,61,74	2.14	20 (35%)	64,98,114	2.94	26 (40%)
29	BCR	C	515	-	41,41,41	1.32	3 (7%)	56,56,56	1.28	6 (10%)
24	CLA	9	612	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
24	CLA	BU	612	22	40,44,73	1.55	11 (27%)	47,76,113	1.49	4 (8%)
24	CLA	0	611	27	59,63,73	1.33	10 (16%)	71,101,113	1.48	10 (14%)
23	CHL	Y	306	8	52,56,74	2.23	18 (34%)	58,92,114	2.95	23 (39%)
24	CLA	BF	511	21	69,73,73	1.26	11 (15%)	83,113,113	1.34	5 (6%)
24	CLA	y	304	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
24	CLA	Au	602	8	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)
24	CLA	BQ	611	27	64,68,73	1.30	7 (10%)	77,107,113	1.36	5 (6%)
23	CHL	s	601	-	50,54,74	2.30	18 (36%)	56,90,114	3.00	21 (37%)
24	CLA	Au	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.43	7 (10%)
24	CLA	BQ	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
27	LHG	G	618	24	48,48,48	0.60	0	51,54,54	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
32	SQD	Az	101	-	41,42,54	1.59	8 (19%)	50,53,65	1.83	9 (18%)
23	CHL	y	310	-	67,71,74	2.08	19 (28%)	75,109,114	2.65	26 (34%)
24	CLA	8	303	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
24	CLA	BF	513	-	69,73,73	1.24	11 (15%)	83,113,113	1.34	6 (7%)
23	CHL	S	601	14	50,54,74	2.26	19 (38%)	56,90,114	3.04	22 (39%)
23	CHL	BV	607	-	50,54,74	2.34	18 (36%)	56,90,114	2.96	23 (41%)
23	CHL	BQ	605	8	52,56,74	2.19	16 (30%)	58,92,114	3.03	20 (34%)
23	CHL	8	307	3	50,54,74	2.28	19 (38%)	56,90,114	3.06	25 (44%)
23	CHL	BU	606	-	57,61,74	2.15	20 (35%)	64,98,114	2.94	25 (39%)
23	CHL	Ba	308	-	67,71,74	1.95	19 (28%)	75,109,114	2.78	26 (34%)
24	CLA	A2	612	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	4 (5%)
23	CHL	6	605	2	50,54,74	2.31	19 (38%)	56,90,114	3.02	22 (39%)
35	BCT	BD	402	-	2,3,3	1.33	0	2,3,3	4.13	1 (50%)
24	CLA	C	509	21	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
24	CLA	7	312	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
26	NEX	r	617	-	38,46,46	1.61	7 (18%)	50,70,70	1.62	9 (18%)
24	CLA	BE	609	4	69,73,73	1.24	9 (13%)	83,113,113	1.44	8 (9%)
24	CLA	BG	402	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	5 (6%)
29	BCR	BD	411	-	41,41,41	1.25	2 (4%)	56,56,56	1.20	5 (8%)
34	DGD	BF	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	7 (9%)
24	CLA	Ba	313	-	64,68,73	1.31	9 (14%)	77,107,113	1.34	7 (9%)
29	BCR	F	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.21	5 (8%)
24	CLA	n	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
26	NEX	n	617	-	38,46,46	1.62	7 (18%)	50,70,70	1.60	9 (18%)
27	LHG	Y	319	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	AA	303	1	65,69,73	1.26	9 (13%)	78,108,113	1.42	7 (8%)
26	NEX	N	617	-	38,46,46	1.57	7 (18%)	50,70,70	1.59	9 (18%)
24	CLA	Au	610	8	68,72,73	1.24	10 (14%)	81,111,113	1.37	7 (8%)
24	CLA	N	614	-	52,56,73	1.46	7 (13%)	62,92,113	1.48	6 (9%)
24	CLA	s	611	-	53,57,73	1.43	10 (18%)	62,93,113	1.45	5 (8%)
28	XAT	5	619	-	39,47,47	6.02	19 (48%)	54,74,74	7.65	35 (64%)
23	CHL	N	608	-	67,71,74	1.95	20 (29%)	75,109,114	2.72	26 (34%)
27	LHG	0	617	24	46,46,48	0.68	1 (2%)	49,52,54	1.33	6 (12%)
24	CLA	v	606	-	69,73,73	1.26	10 (14%)	83,113,113	1.32	7 (8%)
28	XAT	9	619	-	39,47,47	6.07	20 (51%)	54,74,74	7.51	33 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	LUT	BV	614	-	42,43,43	1.66	8 (19%)	51,60,60	1.47	10 (19%)
36	OEX	BD	403	20	0,14,14	-	-	-		
24	CLA	r	602	22	62,66,73	1.32	11 (17%)	72,104,113	1.39	6 (8%)
23	CHL	5	605	1	50,54,74	2.32	19 (38%)	56,90,114	2.99	21 (37%)
24	CLA	5	603	1	59,63,73	1.37	10 (16%)	71,101,113	1.31	8 (11%)
29	BCR	z	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	5 (8%)
24	CLA	g	611	27	64,68,73	1.31	8 (12%)	77,107,113	1.35	6 (7%)
24	CLA	C	507	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	5 (6%)
24	CLA	A2	602	8	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
27	LHG	D	404	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	5 (9%)
29	BCR	z	102	-	41,41,41	1.27	3 (7%)	56,56,56	1.32	8 (14%)
23	CHL	0	601	2	65,69,74	2.02	19 (29%)	72,106,114	2.72	26 (36%)
24	CLA	C	502	21	69,73,73	1.25	10 (14%)	83,113,113	1.28	5 (6%)
23	CHL	Y	307	-	54,58,74	2.08	18 (33%)	59,94,114	3.13	23 (38%)
25	LUT	BQ	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.52	11 (21%)
24	CLA	S	612	14	59,63,73	1.35	9 (15%)	71,101,113	1.41	6 (8%)
38	PHO	A	408	-	58,69,69	2.00	11 (18%)	56,99,99	1.53	9 (16%)
29	BCR	v	622	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	5 (8%)
28	XAT	BB	301	-	39,47,47	6.17	20 (51%)	54,74,74	7.80	34 (62%)
24	CLA	BE	612	4	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
29	BCR	BE	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	5 (8%)
24	CLA	v	610	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
24	CLA	b	610	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	5 (6%)
24	CLA	AA	311	1	52,56,73	1.44	11 (21%)	60,92,113	1.45	8 (13%)
23	CHL	0	608	2	50,54,74	2.27	18 (36%)	56,90,114	3.08	22 (39%)
30	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.37	7 (11%)
23	CHL	G	609	-	60,64,74	2.07	19 (31%)	63,100,114	2.78	23 (36%)
24	CLA	s	603	14	49,53,73	1.50	8 (16%)	59,89,113	1.45	5 (8%)
24	CLA	7	303	1	65,69,73	1.27	9 (13%)	78,108,113	1.41	5 (6%)
24	CLA	G	612	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	6 (7%)
24	CLA	G	611	27	64,68,73	1.32	9 (14%)	77,107,113	1.39	9 (11%)
24	CLA	AA	304	-	59,63,73	1.37	9 (15%)	71,101,113	1.29	6 (8%)
24	CLA	s	602	14	65,69,73	1.30	9 (13%)	78,108,113	1.31	5 (6%)
24	CLA	G	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.44	7 (10%)
24	CLA	Ba	315	-	52,56,73	1.43	9 (17%)	62,92,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHL	A2	601	8	67,71,74	1.93	20 (29%)	75,109,114	2.74	25 (33%)
24	CLA	b	614	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	4 (4%)
24	CLA	Y	315	-	52,56,73	1.42	10 (19%)	62,92,113	1.50	8 (12%)
32	SQD	BO	102	-	41,42,54	1.63	7 (17%)	50,53,65	1.46	7 (14%)
23	CHL	S	605	14	50,54,74	2.21	17 (34%)	56,90,114	3.15	21 (37%)
34	DGD	Av	102	-	63,63,67	0.91	2 (3%)	77,77,81	1.38	9 (11%)
24	CLA	S	602	14	65,69,73	1.28	9 (13%)	78,108,113	1.35	6 (7%)
25	LUT	BJ	615	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	9 (17%)
34	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.38	7 (9%)
25	LUT	AA	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.55	11 (21%)
34	DGD	A	402	-	60,60,67	0.93	2 (3%)	74,74,81	1.38	8 (10%)
24	CLA	BD	410	-	64,68,73	1.29	9 (14%)	77,107,113	1.38	7 (9%)
24	CLA	d	401	5	69,73,73	1.23	11 (15%)	83,113,113	1.33	7 (8%)
24	CLA	1	502	21	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
28	XAT	BJ	619	-	39,47,47	6.17	22 (56%)	54,74,74	7.65	34 (62%)
24	CLA	BV	611	-	53,57,73	1.43	10 (18%)	62,93,113	1.44	5 (8%)
29	BCR	B	623	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	5 (8%)
24	CLA	C	512	-	69,73,73	1.24	11 (15%)	83,113,113	1.33	7 (8%)
27	LHG	b	623	-	45,45,48	0.66	1 (2%)	48,51,54	1.25	4 (8%)
30	LMG	Aw	101	-	40,40,55	0.81	0	48,48,63	1.34	7 (14%)
24	CLA	BB	311	8	64,68,73	1.31	10 (15%)	77,107,113	1.35	5 (6%)
23	CHL	7	308	-	62,66,74	1.99	20 (32%)	68,103,114	2.92	25 (36%)
24	CLA	v	609	4	69,73,73	1.23	11 (15%)	83,113,113	1.31	5 (6%)
24	CLA	b	609	4	69,73,73	1.23	8 (11%)	83,113,113	1.40	7 (8%)
30	LMG	B	624	-	40,40,55	0.84	1 (2%)	48,48,63	1.31	5 (10%)
24	CLA	9	603	-	59,63,73	1.37	10 (16%)	71,101,113	1.31	8 (11%)
28	XAT	BQ	619	-	39,47,47	6.12	21 (53%)	54,74,74	7.75	34 (62%)
25	LUT	6	616	-	42,43,43	1.71	7 (16%)	51,60,60	1.65	10 (19%)
24	CLA	9	602	1	65,69,73	1.29	10 (15%)	78,108,113	1.31	6 (7%)
25	LUT	y	316	-	42,43,43	1.62	8 (19%)	51,60,60	1.47	10 (19%)
26	NEX	A6	616	-	38,46,46	1.63	7 (18%)	50,70,70	1.64	9 (18%)
24	CLA	c	509	21	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
24	CLA	BF	512	21	69,73,73	1.26	11 (15%)	83,113,113	1.38	7 (8%)
24	CLA	s	608	-	49,53,73	1.51	8 (16%)	59,89,113	1.39	4 (6%)
23	CHL	5	609	-	63,67,74	2.17	21 (33%)	70,104,114	2.93	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	BF	509	21	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
28	XAT	AA	301	-	39,47,47	6.20	22 (56%)	54,74,74	7.72	34 (62%)
24	CLA	g	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
25	LUT	BB	317	-	42,43,43	1.67	8 (19%)	51,60,60	1.54	9 (17%)
24	CLA	B	609	-	69,73,73	1.22	10 (14%)	83,113,113	1.31	5 (6%)
24	CLA	s	613	14	53,57,73	1.41	9 (16%)	62,93,113	1.46	6 (9%)
24	CLA	8	308	-	49,53,73	1.48	12 (24%)	59,89,113	1.78	12 (20%)
23	CHL	AB	307	3	50,54,74	2.32	19 (38%)	56,90,114	3.03	22 (39%)
29	BCR	H	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.29	9 (16%)
23	CHL	6	606	-	50,54,74	2.20	20 (40%)	56,90,114	3.11	21 (37%)
24	CLA	c	513	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	6 (7%)
24	CLA	N	613	8	64,68,73	1.30	9 (14%)	77,107,113	1.39	6 (7%)
24	CLA	y	314	8	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
24	CLA	6	613	-	62,66,73	1.35	11 (17%)	74,104,113	1.49	9 (12%)
25	LUT	Y	317	-	42,43,43	1.66	8 (19%)	51,60,60	1.54	10 (19%)
24	CLA	C	504	21	69,73,73	1.23	8 (11%)	83,113,113	1.33	6 (7%)
23	CHL	n	601	8	67,71,74	2.00	17 (25%)	75,109,114	2.68	24 (32%)
24	CLA	1	512	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	8 (9%)
25	LUT	AB	311	-	42,43,43	1.64	8 (19%)	51,60,60	1.61	10 (19%)
28	XAT	n	619	-	39,47,47	6.12	21 (53%)	54,74,74	7.74	34 (62%)
26	NEX	BQ	617	-	38,46,46	1.68	7 (18%)	50,70,70	1.66	9 (18%)
24	CLA	0	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	5 (8%)
26	NEX	G	617	-	38,46,46	1.64	7 (18%)	50,70,70	1.69	9 (18%)
24	CLA	B	606	-	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
31	PL9	2	404	-	55,55,55	1.68	10 (18%)	68,69,69	1.52	13 (19%)
34	DGD	1	518	-	61,61,67	0.90	2 (3%)	75,75,81	1.40	10 (13%)
27	LHG	Ba	319	24	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
24	CLA	N	612	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	4 (5%)
23	CHL	BB	308	-	67,71,74	1.89	19 (28%)	75,109,114	2.81	26 (34%)
33	HEM	F	102	7	50,50,50	1.34	7 (14%)	66,82,82	1.18	6 (9%)
27	LHG	BF	520	-	48,48,48	0.55	0	51,54,54	1.27	6 (11%)
24	CLA	B	612	4	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
32	SQD	D	406	-	49,50,54	1.57	7 (14%)	58,61,65	1.45	7 (12%)
34	DGD	BD	401	-	60,60,67	0.94	2 (3%)	74,74,81	1.38	6 (8%)
23	CHL	BJ	605	8	50,54,74	2.25	16 (32%)	56,90,114	3.11	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
23	CHL	g	606	-	54,58,74	2.19	17 (31%)	59,94,114	3.00	22 (37%)
23	CHL	Ba	309	-	67,71,74	2.01	19 (28%)	75,109,114	2.69	25 (33%)
24	CLA	6	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	5 (8%)
24	CLA	9	613	1	59,63,73	1.35	9 (15%)	71,101,113	1.41	6 (8%)
26	NEX	BB	320	-	38,46,46	1.65	7 (18%)	50,70,70	1.63	10 (20%)
27	LHG	C	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
23	CHL	Ba	310	-	67,71,74	2.09	20 (29%)	75,109,114	2.65	26 (34%)
34	DGD	BF	517	-	56,56,67	0.96	2 (3%)	70,70,81	1.50	11 (15%)
27	LHG	d	404	-	48,48,48	0.65	1 (2%)	51,54,54	1.26	6 (11%)
26	NEX	y	318	-	38,46,46	1.65	7 (18%)	50,70,70	1.62	9 (18%)
24	CLA	BU	602	22	62,66,73	1.33	11 (17%)	72,104,113	1.39	6 (8%)
32	SQD	R	411	-	53,54,54	1.51	7 (13%)	62,65,65	1.34	6 (9%)
23	CHL	BQ	608	-	67,71,74	1.99	19 (28%)	75,109,114	2.69	26 (34%)
23	CHL	BV	606	-	59,63,74	2.05	16 (27%)	64,99,114	3.04	25 (39%)
24	CLA	BV	602	14	65,69,73	1.30	9 (13%)	78,108,113	1.29	5 (6%)
30	LMG	BF	501	-	51,51,55	0.74	0	59,59,63	1.34	7 (11%)
25	LUT	g	615	-	42,43,43	1.61	8 (19%)	51,60,60	1.52	9 (17%)
24	CLA	n	611	27	64,68,73	1.30	7 (10%)	77,107,113	1.37	5 (6%)
24	CLA	BQ	603	8	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
24	CLA	BB	315	-	52,56,73	1.42	10 (19%)	62,92,113	1.50	8 (12%)
24	CLA	c	511	21	69,73,73	1.25	11 (15%)	83,113,113	1.34	5 (6%)
23	CHL	0	609	-	62,66,74	2.20	21 (33%)	68,103,114	3.06	25 (36%)
25	LUT	AA	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.51	10 (19%)
32	SQD	L	103	-	53,54,54	1.52	8 (15%)	62,65,65	1.37	6 (9%)
23	CHL	Au	607	-	67,71,74	1.92	20 (29%)	75,109,114	2.79	27 (36%)
24	CLA	BQ	614	-	52,56,73	1.46	6 (11%)	62,92,113	1.50	8 (12%)
23	CHL	BV	601	-	50,54,74	2.29	18 (36%)	56,90,114	3.00	20 (35%)
24	CLA	9	611	27	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
24	CLA	BU	611	22	53,57,73	1.43	11 (20%)	62,93,113	1.42	5 (8%)
24	CLA	2	403	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	5 (6%)
34	DGD	a	413	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	9 (12%)
23	CHL	A6	607	14	50,54,74	2.36	19 (38%)	56,90,114	3.25	19 (33%)
23	CHL	y	306	8	52,56,74	2.25	19 (36%)	58,92,114	2.93	22 (37%)
24	CLA	1	513	21	69,73,73	1.24	9 (13%)	83,113,113	1.37	6 (7%)
23	CHL	A2	607	-	67,71,74	1.93	20 (29%)	75,109,114	2.82	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	BCR	BE	620	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	4 (7%)
30	LMG	D	405	-	46,46,55	0.77	1 (2%)	54,54,63	1.35	5 (9%)
24	CLA	b	611	-	69,73,73	1.27	9 (13%)	83,113,113	1.61	11 (13%)
24	CLA	A	405	20	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
24	CLA	AA	313	-	49,53,73	1.47	9 (18%)	59,89,113	1.49	7 (11%)
28	XAT	7	301	-	39,47,47	6.21	21 (53%)	54,74,74	7.69	34 (62%)
24	CLA	C	506	21	69,73,73	1.26	11 (15%)	83,113,113	1.30	7 (8%)
24	CLA	g	612	-	64,68,73	1.33	8 (12%)	77,107,113	1.27	5 (6%)
23	CHL	BB	302	8	67,71,74	1.91	19 (28%)	75,109,114	2.81	28 (37%)
24	CLA	S	604	-	54,58,73	1.40	10 (18%)	65,95,113	1.46	5 (7%)
24	CLA	n	614	-	52,56,73	1.46	6 (11%)	62,92,113	1.50	8 (12%)
24	CLA	9	604	-	54,58,73	1.45	11 (20%)	65,95,113	1.55	9 (13%)
24	CLA	A6	602	14	65,69,73	1.27	9 (13%)	78,108,113	1.35	6 (7%)
24	CLA	n	603	8	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
23	CHL	N	601	8	67,71,74	1.93	20 (29%)	75,109,114	2.74	24 (32%)
23	CHL	AA	308	-	62,66,74	2.00	20 (32%)	68,103,114	2.95	26 (38%)
24	CLA	AA	312	-	49,53,73	1.46	8 (16%)	59,89,113	1.49	6 (10%)
34	DGD	1	516	-	56,56,67	0.99	4 (7%)	70,70,81	1.50	11 (15%)
26	NEX	g	617	-	38,46,46	1.65	6 (15%)	50,70,70	1.68	9 (18%)
27	LHG	c	519	-	48,48,48	0.55	0	51,54,54	1.26	6 (11%)
24	CLA	2	402	5	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
24	CLA	Y	303	8	69,73,73	1.25	12 (17%)	83,113,113	1.33	4 (4%)
24	CLA	r	610	27	53,57,73	1.41	11 (20%)	62,93,113	1.44	6 (9%)
23	CHL	BB	309	-	67,71,74	1.92	19 (28%)	75,109,114	2.74	24 (32%)
25	LUT	7	317	-	42,43,43	1.64	8 (19%)	51,60,60	1.50	9 (17%)
26	NEX	S	616	-	38,46,46	1.65	7 (18%)	50,70,70	1.63	9 (18%)
25	LUT	7	316	-	42,43,43	1.68	8 (19%)	51,60,60	1.59	7 (13%)
24	CLA	r	612	22	40,44,73	1.56	11 (27%)	47,76,113	1.49	5 (10%)
23	CHL	6	609	-	62,66,74	2.19	22 (35%)	68,103,114	3.04	24 (35%)
38	PHO	R	408	-	58,69,69	1.95	11 (18%)	56,99,99	1.61	7 (12%)
25	LUT	n	616	-	42,43,43	1.62	8 (19%)	51,60,60	1.53	11 (21%)
24	CLA	v	607	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	4 (4%)
28	XAT	Au	619	-	39,47,47	6.18	21 (53%)	54,74,74	7.66	34 (62%)
24	CLA	Au	603	8	69,73,73	1.23	10 (14%)	83,113,113	1.28	4 (4%)
27	LHG	y	319	24	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	C	513	21	69,73,73	1.24	9 (13%)	83,113,113	1.36	5 (6%)
27	LHG	r	618	24	41,41,48	0.72	1 (2%)	44,47,54	1.34	7 (15%)
23	CHL	S	607	-	50,54,74	2.23	18 (36%)	56,90,114	3.26	22 (39%)
24	CLA	s	609	14	59,63,73	1.35	9 (15%)	71,101,113	1.40	7 (9%)
29	BCR	1	515	-	41,41,41	1.35	4 (9%)	56,56,56	1.28	6 (10%)
24	CLA	A2	611	27	64,68,73	1.28	9 (14%)	77,107,113	1.35	7 (9%)
24	CLA	C	503	21	69,73,73	1.25	10 (14%)	83,113,113	1.33	6 (7%)
25	LUT	BB	316	-	42,43,43	1.66	8 (19%)	51,60,60	1.53	11 (21%)
23	CHL	AB	304	3	50,54,74	2.27	19 (38%)	56,90,114	2.98	22 (39%)
23	CHL	G	601	8	67,71,74	1.93	20 (29%)	75,109,114	2.77	28 (37%)
24	CLA	6	614	2	52,56,73	1.43	10 (19%)	62,92,113	1.39	6 (9%)
24	CLA	b	604	4	69,73,73	1.23	9 (13%)	83,113,113	1.30	4 (4%)
27	LHG	1	521	-	48,48,48	0.61	0	51,54,54	1.27	6 (11%)
30	LMG	i	101	-	48,48,55	0.74	1 (2%)	56,56,63	1.32	6 (10%)
29	BCR	Bb	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.33	9 (16%)
32	SQD	A	413	-	53,54,54	1.51	7 (13%)	62,65,65	1.33	6 (9%)
29	BCR	B	617	-	41,41,41	1.22	2 (4%)	56,56,56	1.34	8 (14%)
24	CLA	c	508	-	69,73,73	1.25	11 (15%)	83,113,113	1.29	5 (6%)
25	LUT	8	311	-	42,43,43	1.59	8 (19%)	51,60,60	1.41	9 (17%)
26	NEX	BJ	617	-	38,46,46	1.66	6 (15%)	50,70,70	1.69	9 (18%)
24	CLA	0	604	-	49,53,73	1.47	9 (18%)	59,89,113	1.43	6 (10%)
32	SQD	BG	406	-	49,50,54	1.58	7 (14%)	58,61,65	1.44	7 (12%)
23	CHL	n	607	-	67,71,74	1.96	18 (26%)	75,109,114	2.78	24 (32%)
23	CHL	y	307	-	54,58,74	2.20	19 (35%)	59,94,114	2.96	23 (38%)
24	CLA	Ba	304	-	69,73,73	1.27	8 (11%)	83,113,113	1.25	5 (6%)
23	CHL	5	608	-	50,54,74	2.26	20 (40%)	56,90,114	3.03	20 (35%)
30	LMG	c	501	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
25	LUT	s	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.52	11 (21%)
29	BCR	Ay	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	7 (12%)
23	CHL	9	607	-	64,68,74	1.96	19 (29%)	71,105,114	2.79	25 (35%)
24	CLA	A	407	-	54,58,73	1.41	11 (20%)	65,95,113	1.50	9 (13%)
24	CLA	r	609	22	69,73,73	1.24	11 (15%)	83,113,113	1.36	6 (7%)
23	CHL	9	608	-	50,54,74	2.26	20 (40%)	56,90,114	3.02	20 (35%)
23	CHL	s	607	-	50,54,74	2.34	18 (36%)	56,90,114	2.96	23 (41%)
24	CLA	6	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.69	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	BU	610	27	53,57,73	1.40	11 (20%)	62,93,113	1.45	6 (9%)
24	CLA	n	602	8	69,73,73	1.26	8 (11%)	83,113,113	1.25	6 (7%)
25	LUT	Ba	316	-	42,43,43	1.62	8 (19%)	51,60,60	1.46	9 (17%)
27	LHG	1	520	-	48,48,48	0.57	0	51,54,54	1.26	6 (11%)
29	BCR	b	601	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	8 (14%)
24	CLA	BF	514	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	4 (4%)
24	CLA	BE	611	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
24	CLA	R	406	-	54,58,73	1.40	12 (22%)	65,95,113	1.49	8 (12%)
29	BCR	v	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.34	8 (14%)
24	CLA	Y	312	-	64,68,73	1.29	10 (15%)	77,107,113	1.38	9 (11%)
24	CLA	b	606	4	69,73,73	1.26	10 (14%)	83,113,113	1.27	6 (7%)
24	CLA	A2	604	-	54,58,73	1.39	10 (18%)	65,95,113	1.48	6 (9%)
24	CLA	BE	604	4	69,73,73	1.23	9 (13%)	83,113,113	1.31	4 (4%)
23	CHL	AB	306	-	50,54,74	2.34	20 (40%)	56,90,114	2.95	23 (41%)
24	CLA	BJ	610	8	68,72,73	1.27	7 (10%)	81,111,113	1.29	7 (8%)
28	XAT	G	619	-	39,47,47	6.18	22 (56%)	54,74,74	7.66	34 (62%)
29	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	5 (8%)
34	DGD	R	401	-	60,60,67	0.92	2 (3%)	74,74,81	1.38	8 (10%)
24	CLA	y	303	8	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	s	612	14	59,63,73	1.36	9 (15%)	71,101,113	1.37	6 (8%)
23	CHL	Y	302	8	67,71,74	1.92	20 (29%)	75,109,114	2.79	27 (36%)
30	LMG	b	621	-	51,51,55	0.72	0	59,59,63	1.39	7 (11%)
23	CHL	BB	310	-	67,71,74	1.94	19 (28%)	75,109,114	2.71	23 (30%)
27	LHG	5	618	24	40,40,48	0.64	1 (2%)	43,46,54	1.30	6 (13%)
23	CHL	Ba	302	8	67,71,74	1.98	19 (28%)	75,109,114	2.74	27 (36%)
24	CLA	BB	305	-	54,58,73	1.42	10 (18%)	65,95,113	1.46	7 (10%)
24	CLA	A6	603	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	4 (6%)
25	LUT	s	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.46	11 (21%)
25	LUT	G	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.64	11 (21%)
24	CLA	8	310	-	49,53,73	1.51	9 (18%)	59,89,113	1.53	6 (10%)
23	CHL	A6	606	-	59,63,74	2.06	19 (32%)	64,99,114	3.02	25 (39%)
24	CLA	n	613	-	64,68,73	1.33	10 (15%)	77,107,113	1.34	6 (7%)
24	CLA	BE	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	4 (4%)
23	CHL	BB	307	-	54,58,74	2.08	18 (33%)	59,94,114	3.12	23 (38%)
24	CLA	G	603	8	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
28	XAT	g	619	-	39,47,47	6.17	22 (56%)	54,74,74	7.66	34 (62%)
24	CLA	5	604	-	54,58,73	1.44	10 (18%)	65,95,113	1.54	9 (13%)
31	PL9	D	403	-	55,55,55	1.80	9 (16%)	68,69,69	1.49	11 (16%)
24	CLA	BE	606	4	69,73,73	1.26	10 (14%)	83,113,113	1.28	6 (7%)
23	CHL	BJ	606	-	54,58,74	2.18	18 (33%)	59,94,114	3.00	24 (40%)
27	LHG	b	622	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
33	HEM	4	102	7	50,50,50	1.33	6 (12%)	66,82,82	1.18	6 (9%)
24	CLA	BQ	613	-	64,68,73	1.32	10 (15%)	77,107,113	1.34	6 (7%)
24	CLA	Ba	314	8	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
24	CLA	1	504	21	69,73,73	1.23	10 (14%)	83,113,113	1.34	5 (6%)
23	CHL	g	605	8	50,54,74	2.25	16 (32%)	56,90,114	3.12	23 (41%)
24	CLA	g	603	8	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
27	LHG	BE	623	-	45,45,48	0.68	1 (2%)	48,51,54	1.25	4 (8%)
30	LMG	BE	621	-	51,51,55	0.72	1 (1%)	59,59,63	1.40	8 (13%)
24	CLA	6	610	2	64,68,73	1.30	10 (15%)	77,107,113	1.56	11 (14%)
24	CLA	a	410	-	64,68,73	1.29	9 (14%)	77,107,113	1.38	7 (9%)
23	CHL	AA	310	-	62,66,74	2.14	19 (30%)	68,103,114	2.89	27 (39%)
24	CLA	b	607	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
29	BCR	A	411	-	41,41,41	1.27	3 (7%)	56,56,56	1.25	6 (10%)
24	CLA	a	406	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
23	CHL	s	605	14	50,54,74	2.28	18 (36%)	56,90,114	3.00	24 (42%)
24	CLA	5	610	1	60,64,73	1.35	12 (20%)	72,102,113	1.39	9 (12%)
36	OEX	a	403	20	0,14,14	-	-	-		
32	SQD	l	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.36	6 (9%)
24	CLA	b	608	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
25	LUT	A6	615	-	42,43,43	1.62	8 (19%)	51,60,60	1.75	14 (27%)
34	DGD	c	516	-	56,56,67	0.97	2 (3%)	70,70,81	1.50	12 (17%)
24	CLA	1	505	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
25	LUT	Au	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.65	11 (21%)
24	CLA	r	603	22	64,68,73	1.31	10 (15%)	77,107,113	1.29	5 (6%)
24	CLA	BE	610	-	69,73,73	1.23	10 (14%)	83,113,113	1.32	5 (6%)
25	LUT	A2	615	-	42,43,43	1.67	8 (19%)	51,60,60	1.53	10 (19%)
27	LHG	BE	622	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	B	605	4	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
24	CLA	BB	313	-	64,68,73	1.30	11 (17%)	77,107,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHL	Au	606	-	54,58,74	2.15	20 (37%)	59,94,114	2.99	23 (38%)
24	CLA	r	608	22	62,66,73	1.32	10 (16%)	74,104,113	1.41	4 (5%)
23	CHL	BQ	606	8	54,58,74	2.20	19 (35%)	59,94,114	2.94	23 (38%)
38	PHO	BD	408	-	58,69,69	2.00	11 (18%)	56,99,99	1.53	8 (14%)
23	CHL	A2	606	8	54,58,74	2.16	19 (35%)	59,94,114	3.00	22 (37%)
23	CHL	r	607	22	62,66,74	1.98	20 (32%)	68,103,114	2.90	26 (38%)
23	CHL	Ba	306	8	52,56,74	2.24	19 (36%)	58,92,114	2.93	21 (36%)
24	CLA	BV	609	14	59,63,73	1.35	8 (13%)	71,101,113	1.40	6 (8%)
24	CLA	AA	305	-	49,53,73	1.48	10 (20%)	59,89,113	1.42	7 (11%)
24	CLA	B	607	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	4 (4%)
24	CLA	c	510	21	69,73,73	1.26	11 (15%)	83,113,113	1.32	6 (7%)
24	CLA	B	615	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
36	OEX	R	402	20	0,14,14	-	-	-		
24	CLA	6	611	27	59,63,73	1.33	10 (16%)	71,101,113	1.49	10 (14%)
24	CLA	A6	608	-	49,53,73	1.47	9 (18%)	59,89,113	1.42	6 (10%)
24	CLA	BJ	603	8	69,73,73	1.26	8 (11%)	83,113,113	1.29	4 (4%)
24	CLA	1	503	21	69,73,73	1.26	11 (15%)	83,113,113	1.34	6 (7%)
25	LUT	9	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.69	9 (17%)
23	CHL	n	606	8	54,58,74	2.18	19 (35%)	59,94,114	2.96	23 (38%)
23	CHL	BQ	601	8	67,71,74	1.99	17 (25%)	75,109,114	2.68	24 (32%)
24	CLA	N	611	27	64,68,73	1.29	9 (14%)	77,107,113	1.35	7 (9%)
25	LUT	BU	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.55	11 (21%)
30	LMG	v	620	-	51,51,55	0.72	0	59,59,63	1.38	7 (11%)
32	SQD	l	102	-	41,42,54	1.63	7 (17%)	50,53,65	1.45	7 (14%)
29	BCR	h	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
23	CHL	9	605	1	50,54,74	2.31	19 (38%)	56,90,114	3.00	21 (37%)
24	CLA	G	602	8	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
24	CLA	1	506	21	69,73,73	1.26	12 (17%)	83,113,113	1.30	7 (8%)
24	CLA	BF	505	-	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)
24	CLA	B	611	4	69,73,73	1.24	10 (14%)	83,113,113	1.40	7 (8%)
24	CLA	v	603	4	69,73,73	1.23	9 (13%)	83,113,113	1.31	5 (6%)
24	CLA	BF	510	21	69,73,73	1.27	11 (15%)	83,113,113	1.33	7 (8%)
27	LHG	2	405	-	45,45,48	0.68	1 (2%)	48,51,54	1.23	4 (8%)
31	PL9	d	403	-	55,55,55	1.65	9 (16%)	68,69,69	1.66	14 (20%)
23	CHL	BV	605	14	50,54,74	2.27	18 (36%)	56,90,114	2.99	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	B	604	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
28	XAT	r	616	-	39,47,47	6.05	20 (51%)	54,74,74	7.70	38 (70%)
24	CLA	v	611	4	69,73,73	1.24	10 (14%)	83,113,113	1.39	7 (8%)
23	CHL	BU	607	22	62,66,74	1.99	20 (32%)	68,103,114	2.91	26 (38%)
23	CHL	6	601	2	65,69,74	2.02	19 (29%)	72,106,114	2.72	27 (37%)
25	LUT	A6	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	10 (19%)
26	NEX	A2	617	-	38,46,46	1.85	9 (23%)	50,70,70	1.70	10 (20%)
24	CLA	BV	612	14	59,63,73	1.36	9 (15%)	71,101,113	1.37	6 (8%)
24	CLA	Y	304	8	69,73,73	1.26	11 (15%)	83,113,113	1.30	6 (7%)
26	NEX	Au	617	-	38,46,46	1.64	6 (15%)	50,70,70	1.69	9 (18%)
29	BCR	K	102	-	41,41,41	1.25	3 (7%)	56,56,56	1.30	8 (14%)
24	CLA	BU	609	22	69,73,73	1.24	11 (15%)	83,113,113	1.36	6 (7%)
23	CHL	7	310	-	62,66,74	2.13	19 (30%)	68,103,114	2.88	27 (39%)
24	CLA	AB	308	-	49,53,73	1.50	11 (22%)	59,89,113	1.72	13 (22%)
28	XAT	A2	619	-	39,47,47	6.09	20 (51%)	54,74,74	7.74	35 (64%)
24	CLA	BG	401	5	69,73,73	1.23	11 (15%)	83,113,113	1.35	7 (8%)
34	DGD	C	518	-	61,61,67	0.90	2 (3%)	75,75,81	1.40	10 (13%)
25	LUT	BJ	616	-	42,43,43	1.65	7 (16%)	51,60,60	1.65	9 (17%)
29	BCR	a	411	-	41,41,41	1.23	2 (4%)	56,56,56	1.19	5 (8%)
24	CLA	A2	603	8	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
23	CHL	G	607	-	67,71,74	1.93	20 (29%)	75,109,114	2.79	25 (33%)
29	BCR	BF	516	-	41,41,41	1.37	3 (7%)	56,56,56	1.31	8 (14%)
24	CLA	6	603	-	59,63,73	1.35	12 (20%)	71,101,113	1.35	7 (9%)
23	CHL	Y	308	-	67,71,74	1.89	19 (28%)	75,109,114	2.81	26 (34%)
23	CHL	BQ	609	-	67,71,74	1.99	18 (26%)	75,109,114	2.67	26 (34%)
24	CLA	7	311	1	52,56,73	1.42	11 (21%)	60,92,113	1.44	8 (13%)
30	LMG	2	407	-	46,46,55	0.78	1 (2%)	54,54,63	1.35	5 (9%)
23	CHL	5	601	1	50,54,74	2.27	20 (40%)	56,90,114	3.15	22 (39%)
24	CLA	1	509	21	69,73,73	1.25	11 (15%)	83,113,113	1.35	9 (10%)
24	CLA	B	614	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	6 (7%)
25	LUT	9	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.65	11 (21%)
29	BCR	k	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.24	6 (10%)
32	SQD	L	101	-	41,42,54	1.62	7 (17%)	50,53,65	1.57	9 (18%)
24	CLA	7	314	1	49,53,73	1.48	10 (20%)	59,89,113	1.48	5 (8%)
24	CLA	BE	616	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
28	XAT	y	301	-	39,47,47	6.11	22 (56%)	54,74,74	7.77	34 (62%)
24	CLA	BE	607	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
25	LUT	g	616	-	42,43,43	1.65	7 (16%)	51,60,60	1.59	10 (19%)
24	CLA	N	604	-	54,58,73	1.39	10 (18%)	65,95,113	1.48	6 (9%)
25	LUT	0	615	-	42,43,43	1.69	8 (19%)	51,60,60	1.48	10 (19%)
24	CLA	BJ	614	8	52,56,73	1.44	7 (13%)	62,92,113	1.46	4 (6%)
24	CLA	BB	304	8	69,73,73	1.26	11 (15%)	83,113,113	1.30	6 (7%)
29	BCR	BK	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	9 (16%)
23	CHL	Ba	307	-	54,58,74	2.19	19 (35%)	59,94,114	2.97	23 (38%)
23	CHL	N	609	8	67,71,74	1.94	19 (28%)	75,109,114	2.71	21 (28%)
24	CLA	A6	610	-	60,64,73	1.34	10 (16%)	72,102,113	1.38	5 (6%)
29	BCR	b	620	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	4 (7%)
24	CLA	G	613	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
30	LMG	BG	405	-	46,46,55	0.78	1 (2%)	54,54,63	1.34	5 (9%)
24	CLA	v	612	4	69,73,73	1.25	11 (15%)	83,113,113	1.35	8 (9%)
24	CLA	A6	612	14	59,63,73	1.34	9 (15%)	71,101,113	1.43	6 (8%)
27	LHG	BB	319	-	48,48,48	0.67	1 (2%)	51,54,54	1.27	6 (11%)
24	CLA	r	611	22	53,57,73	1.43	11 (20%)	62,93,113	1.42	5 (8%)
27	LHG	BU	617	24	41,41,48	0.74	1 (2%)	44,47,54	1.35	7 (15%)
27	LHG	W	201	-	48,48,48	0.60	0	51,54,54	1.26	6 (11%)
34	DGD	BK	102	-	63,63,67	0.95	3 (4%)	77,77,81	1.47	10 (12%)
34	DGD	1	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.44	8 (10%)
24	CLA	0	602	2	64,68,73	1.28	11 (17%)	77,107,113	1.35	8 (10%)
24	CLA	c	502	21	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	7	305	-	49,53,73	1.49	9 (18%)	59,89,113	1.42	7 (11%)
24	CLA	AB	303	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	4 (6%)
24	CLA	A6	611	-	53,57,73	1.42	10 (18%)	62,93,113	1.41	5 (8%)
24	CLA	BF	502	21	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	g	613	-	69,73,73	1.27	8 (11%)	83,113,113	1.32	6 (7%)
28	XAT	7	318	-	39,47,47	6.13	21 (53%)	54,74,74	7.80	34 (62%)
23	CHL	BJ	609	-	62,66,74	2.19	20 (32%)	68,103,114	2.86	24 (35%)
29	BCR	K	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.34	5 (8%)
25	LUT	BQ	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.51	9 (17%)
34	DGD	C	516	-	56,56,67	0.96	2 (3%)	70,70,81	1.49	10 (14%)
29	BCR	BE	601	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHL	6	607	-	57,61,74	2.11	20 (35%)	64,98,114	2.91	25 (39%)
24	CLA	b	605	4	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
35	BCT	2	401	-	2,3,3	1.31	0	2,3,3	3.99	1 (50%)
29	BCR	v	619	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	6 (10%)
23	CHL	A6	605	14	50,54,74	2.20	19 (38%)	56,90,114	3.15	21 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	y	311	8	-	12/33/109/115	-
24	CLA	BU	604	-	-	11/19/95/115	-
28	XAT	Y	301	-	-	18/31/93/93	0/4/4/4
25	LUT	n	615	-	-	1/29/67/67	0/2/2/2
23	CHL	n	608	-	-	13/35/111/117	-
27	LHG	BQ	618	24	-	20/53/53/53	-
23	CHL	5	607	-	-	19/32/108/117	-
24	CLA	BU	601	22	-	10/20/96/115	-
29	BCR	B	618	-	-	7/29/63/63	0/2/2/2
29	BCR	BI	101	-	-	11/29/63/63	0/2/2/2
23	CHL	G	608	-	-	23/35/111/117	-
24	CLA	B	602	4	-	15/39/115/115	-
24	CLA	BJ	613	-	-	13/39/115/115	-
25	LUT	y	317	-	-	1/29/67/67	0/2/2/2
24	CLA	c	512	21	-	12/39/115/115	-
23	CHL	n	605	8	-	6/20/96/117	-
24	CLA	BU	614	-	-	9/15/91/115	-
24	CLA	7	315	1	-	4/15/91/115	-
32	SQD	A1	101	-	-	19/49/69/69	0/1/1/1
23	CHL	BB	306	8	-	7/20/96/117	-
23	CHL	AA	302	1	-	6/17/93/117	-
23	CHL	A6	601	14	-	5/17/93/117	-
24	CLA	n	612	-	-	6/33/109/115	-
23	CHL	n	609	-	-	15/35/111/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	XAT	AB	312	-	-	16/31/93/93	0/4/4/4
24	CLA	C	511	21	-	13/39/115/115	-
28	XAT	8	312	-	-	16/31/93/93	0/4/4/4
26	NEX	BB	318	-	-	10/27/83/83	0/3/3/3
24	CLA	AB	309	-	-	5/15/91/115	-
26	NEX	AA	319	-	-	22/27/83/83	0/3/3/3
24	CLA	8	309	-	-	5/15/91/115	-
34	DGD	h	102	-	-	15/51/91/95	0/2/2/2
38	PHO	a	408	-	-	6/37/103/103	0/5/6/6
23	CHL	Au	605	8	-	7/17/93/117	-
26	NEX	BV	616	-	-	15/27/83/83	0/3/3/3
24	CLA	v	608	4	-	13/39/115/115	-
24	CLA	BV	610	-	-	12/29/105/115	-
25	LUT	S	614	-	-	2/29/67/67	0/2/2/2
28	XAT	BU	616	-	-	17/31/93/93	0/4/4/4
24	CLA	v	602	4	-	15/39/115/115	-
24	CLA	C	510	21	-	16/39/115/115	-
24	CLA	D	401	5	-	18/39/115/115	-
29	BCR	BN	101	-	-	11/29/63/63	0/2/2/2
30	LMG	C	501	-	-	18/46/66/70	0/1/1/1
24	CLA	S	609	14	-	2/21/99/115	-
24	CLA	Au	614	-	-	5/19/95/115	-
29	BCR	8	313	-	-	16/29/63/63	0/2/2/2
32	SQD	2	408	-	-	24/45/65/69	0/1/1/1
24	CLA	BE	603	4	-	16/39/115/115	-
23	CHL	BU	613	22	-	4/12/88/117	-
23	CHL	Au	609	8	-	8/23/101/117	-
23	CHL	7	309	-	-	10/17/93/117	-
29	BCR	C	514	-	-	3/29/63/63	0/2/2/2
27	LHG	C	520	-	-	25/53/53/53	-
24	CLA	Au	612	-	-	10/33/109/115	-
25	LUT	Ba	317	-	-	1/29/67/67	0/2/2/2
23	CHL	BJ	608	-	-	21/35/111/117	-
24	CLA	y	312	27	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PHO	a	409	-	-	15/37/103/103	0/5/6/6
24	CLA	v	604	4	-	14/39/115/115	-
24	CLA	BU	608	22	-	13/31/107/115	-
25	LUT	Au	616	-	-	2/29/67/67	0/2/2/2
25	LUT	N	615	-	-	1/29/67/67	0/2/2/2
27	LHG	g	618	24	-	18/53/53/53	-
24	CLA	BJ	612	-	-	6/33/109/115	-
23	CHL	y	302	8	-	14/35/111/117	-
25	LUT	S	615	-	-	0/29/67/67	0/2/2/2
24	CLA	5	611	27	-	8/15/91/115	-
27	LHG	b	624	-	-	19/53/53/53	-
23	CHL	e	601	-	-	3/15/91/117	-
23	CHL	g	608	-	-	21/35/111/117	-
24	CLA	b	602	-	-	16/39/115/115	-
23	CHL	S	606	-	-	8/26/102/117	-
24	CLA	A2	610	-	-	15/39/115/115	-
23	CHL	9	606	1	-	5/17/93/117	-
27	LHG	A0	202	-	-	14/53/53/53	-
24	CLA	Y	311	8	-	12/33/109/115	-
23	CHL	A2	605	8	-	9/20/96/117	-
24	CLA	b	617	4	-	18/39/115/115	-
24	CLA	v	616	4	-	17/39/115/115	-
26	NEX	Ba	318	-	-	13/27/83/83	0/3/3/3
23	CHL	N	605	8	-	9/20/96/117	-
24	CLA	N	603	8	-	13/39/115/115	-
23	CHL	BJ	601	8	-	17/35/111/117	-
25	LUT	5	615	-	-	3/29/67/67	0/2/2/2
27	LHG	w	201	-	-	16/53/53/53	-
23	CHL	8	305	-	-	9/17/93/117	-
24	CLA	BB	312	-	-	13/33/109/115	-
24	CLA	g	604	-	-	9/21/97/115	-
27	LHG	BJ	618	24	-	18/53/53/53	-
24	CLA	B	616	4	-	17/39/115/115	-
24	CLA	B	603	4	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	BF	521	-	-	22/53/53/53	-
23	CHL	N	607	-	-	14/35/111/117	-
24	CLA	A2	614	-	-	8/19/95/115	-
24	CLA	BQ	610	8	-	14/39/115/115	-
23	CHL	9	601	1	-	9/17/93/117	-
30	LMG	1	519	-	-	22/46/66/70	0/1/1/1
38	PHO	A	409	-	-	16/37/103/103	0/5/6/6
24	CLA	BQ	612	-	-	6/33/109/115	-
27	LHG	9	618	24	-	18/45/45/53	-
29	BCR	AB	313	-	-	16/29/63/63	0/2/2/2
32	SQD	BD	412	-	-	28/49/69/69	0/1/1/1
23	CHL	Au	601	8	-	17/35/111/117	-
24	CLA	c	507	21	-	19/39/115/115	-
24	CLA	C	508	21	-	15/39/115/115	-
23	CHL	Y	309	-	-	14/35/111/117	-
29	BCR	R	410	-	-	5/29/63/63	0/2/2/2
24	CLA	R	404	20	-	10/39/115/115	-
24	CLA	BF	507	21	-	19/39/115/115	-
29	BCR	BF	515	-	-	3/29/63/63	0/2/2/2
23	CHL	Y	310	8	-	17/35/111/117	-
24	CLA	BE	602	-	-	15/39/115/115	-
24	CLA	AB	301	3	-	5/9/81/115	-
23	CHL	8	304	-	-	9/17/93/117	-
24	CLA	S	610	-	-	11/29/105/115	-
24	CLA	g	614	8	-	5/19/95/115	-
24	CLA	BU	603	22	-	8/33/109/115	-
25	LUT	A2	616	-	-	1/29/67/67	0/2/2/2
32	SQD	BO	101	-	-	21/49/69/69	0/1/1/1
24	CLA	BE	615	-	-	18/39/115/115	-
24	CLA	y	313	-	-	12/33/109/115	-
26	NEX	7	319	-	-	22/27/83/83	0/3/3/3
24	CLA	1	510	21	-	16/39/115/115	-
24	CLA	D	402	-	-	12/39/115/115	-
24	CLA	S	603	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	8	306	-	-	6/17/93/117	-
24	CLA	b	613	4	-	15/39/115/115	-
27	LHG	B	621	-	-	23/53/53/53	-
23	CHL	0	606	-	-	7/17/93/117	-
24	CLA	AB	302	-	-	6/15/91/115	-
25	LUT	5	616	-	-	2/29/67/67	0/2/2/2
24	CLA	Y	305	-	-	11/21/97/115	-
24	CLA	r	614	-	-	9/15/91/115	-
23	CHL	y	308	-	-	20/35/111/117	-
23	CHL	g	609	-	-	10/29/105/117	-
24	CLA	n	610	8	-	14/39/115/115	-
24	CLA	B	608	4	-	13/39/115/115	-
29	BCR	1	514	-	-	3/29/63/63	0/2/2/2
25	LUT	r	615	-	-	3/29/67/67	0/2/2/2
30	LMG	1	501	-	-	18/46/66/70	0/1/1/1
30	LMG	A0	201	-	-	16/43/63/70	0/1/1/1
24	CLA	6	602	2	-	18/33/109/115	-
24	CLA	I	102	-	-	14/39/115/115	-
24	CLA	BV	604	-	-	7/21/97/115	-
24	CLA	Ba	303	8	-	15/39/115/115	-
24	CLA	c	503	21	-	15/39/115/115	-
23	CHL	r	605	22	-	22/35/111/117	-
24	CLA	5	614	1	-	6/15/91/115	-
24	CLA	Au	613	-	-	12/39/115/115	-
25	LUT	G	616	-	-	2/29/67/67	0/2/2/2
24	CLA	BE	613	-	-	16/39/115/115	-
24	CLA	5	602	1	-	15/35/111/115	-
24	CLA	v	605	4	-	23/39/115/115	-
24	CLA	AA	315	1	-	3/15/91/115	-
24	CLA	R	405	-	-	6/39/115/115	-
24	CLA	BB	303	8	-	23/39/115/115	-
24	CLA	BE	617	4	-	17/39/115/115	-
27	LHG	c	520	-	-	22/53/53/53	-
34	DGD	a	401	-	-	21/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	s	610	-	-	12/29/105/115	-
24	CLA	1	511	21	-	14/39/115/115	-
23	CHL	7	302	1	-	6/17/93/117	-
24	CLA	g	610	8	-	20/38/114/115	-
24	CLA	7	304	-	-	12/27/103/115	-
24	CLA	BE	608	-	-	19/39/115/115	-
29	BCR	b	618	-	-	3/29/63/63	0/2/2/2
23	CHL	G	605	8	-	7/17/93/117	-
23	CHL	s	606	-	-	8/26/102/117	-
29	BCR	f	101	-	-	11/29/63/63	0/2/2/2
24	CLA	BV	603	14	-	6/15/91/115	-
24	CLA	Ba	311	8	-	12/33/109/115	-
24	CLA	C	505	-	-	8/39/115/115	-
33	HEM	BI	102	6,7	-	3/14/54/54	-
24	CLA	9	614	1	-	6/15/91/115	-
30	LMG	I	101	-	-	12/35/55/70	0/1/1/1
24	CLA	BD	407	-	-	8/21/97/115	-
24	CLA	G	614	-	-	5/19/95/115	-
30	LMG	d	405	-	-	14/41/61/70	0/1/1/1
24	CLA	A6	609	14	-	3/21/99/115	-
23	CHL	9	609	-	-	13/31/107/117	-
28	XAT	N	619	-	-	17/31/93/93	0/4/4/4
24	CLA	AA	314	1	-	7/15/91/115	-
25	LUT	N	616	-	-	1/29/67/67	0/2/2/2
23	CHL	AA	307	1	-	6/17/93/117	-
24	CLA	Ba	312	27	-	14/33/109/115	-
24	CLA	R	409	-	-	11/33/109/115	-
24	CLA	b	603	4	-	14/39/115/115	-
29	BCR	4	101	-	-	8/29/63/63	0/2/2/2
24	CLA	B	601	-	-	15/39/115/115	-
24	CLA	S	608	-	-	6/15/91/115	-
23	CHL	5	606	1	-	6/17/93/117	-
27	LHG	v	621	-	-	23/53/53/53	-
24	CLA	BF	503	21	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	BE	618	-	-	4/29/63/63	0/2/2/2
24	CLA	b	616	-	-	12/39/115/115	-
34	DGD	C	517	-	-	20/51/91/95	0/2/2/2
24	CLA	Ba	305	-	-	9/21/97/115	-
30	LMG	BF	519	-	-	22/46/66/70	0/1/1/1
23	CHL	Au	608	-	-	22/35/111/117	-
25	LUT	6	615	-	-	2/29/67/67	0/2/2/2
24	CLA	A2	613	8	-	12/33/109/115	-
24	CLA	a	407	-	-	8/21/97/115	-
24	CLA	c	504	21	-	22/39/115/115	-
29	BCR	B	619	-	-	6/29/63/63	0/2/2/2
24	CLA	8	302	-	-	6/15/91/115	-
24	CLA	b	612	4	-	12/39/115/115	-
24	CLA	BF	504	21	-	17/39/115/115	-
38	PHO	BD	409	-	-	15/37/103/103	0/5/6/6
23	CHL	BH	601	-	-	2/15/91/117	-
25	LUT	0	616	-	-	1/29/67/67	0/2/2/2
24	CLA	5	613	1	-	8/27/103/115	-
24	CLA	a	405	20	-	9/39/115/115	-
24	CLA	Au	611	27	-	11/33/109/115	-
27	LHG	n	618	24	-	20/53/53/53	-
30	LMG	BL	101	-	-	17/43/63/70	0/1/1/1
23	CHL	AB	305	-	-	9/17/93/117	-
24	CLA	S	611	-	-	6/20/96/115	-
23	CHL	G	606	-	-	9/22/98/117	-
23	CHL	BQ	607	-	-	16/35/111/117	-
34	DGD	c	517	-	-	21/51/91/95	0/2/2/2
23	CHL	AA	306	1	-	5/17/93/117	-
24	CLA	N	610	-	-	16/39/115/115	-
28	XAT	Ba	301	-	-	15/31/93/93	0/4/4/4
31	PL9	BG	403	-	-	8/53/73/73	0/1/1/1
23	CHL	0	605	2	-	5/17/93/117	-
24	CLA	0	603	-	-	8/27/103/115	-
24	CLA	y	315	-	-	6/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	310	-	-	5/15/91/115	-
24	CLA	BD	405	20	-	9/39/115/115	-
30	LMG	c	518	-	-	23/46/66/70	0/1/1/1
24	CLA	B	610	-	-	15/39/115/115	-
23	CHL	g	601	8	-	16/35/111/117	-
25	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
24	CLA	Y	313	-	-	11/33/109/115	-
24	CLA	A6	604	-	-	9/21/97/115	-
24	CLA	BV	608	-	-	7/15/91/115	-
24	CLA	BJ	602	8	-	15/39/115/115	-
23	CHL	0	607	-	-	12/26/102/117	-
24	CLA	BF	508	-	-	15/39/115/115	-
24	CLA	1	508	21	-	16/39/115/115	-
24	CLA	0	614	2	-	11/19/95/115	-
24	CLA	r	604	-	-	9/19/95/115	-
23	CHL	6	608	2	-	7/17/93/117	-
24	CLA	BQ	602	8	-	16/39/115/115	-
30	LMG	v	623	-	-	16/35/55/70	0/1/1/1
27	LHG	Au	618	24	-	17/53/53/53	-
26	NEX	5	617	-	-	17/27/83/83	0/3/3/3
23	CHL	AA	309	-	-	10/17/93/117	-
24	CLA	5	612	-	-	8/15/91/115	-
24	CLA	7	313	-	-	6/15/91/115	-
24	CLA	Aw	102	-	-	14/39/115/115	-
24	CLA	S	613	14	-	9/20/96/115	-
24	CLA	r	601	22	-	10/20/96/115	-
27	LHG	A2	618	24	-	17/53/53/53	-
29	BCR	c	515	-	-	6/29/63/63	0/2/2/2
24	CLA	s	604	-	-	7/21/97/115	-
24	CLA	A	410	-	-	10/33/109/115	-
27	LHG	BE	624	-	-	19/53/53/53	-
24	CLA	v	614	-	-	20/39/115/115	-
24	CLA	Y	314	8	-	14/39/115/115	-
33	HEM	f	102	6,7	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	406	-	-	6/39/115/115	-
23	CHL	BJ	607	-	-	18/35/111/117	-
24	CLA	N	602	8	-	15/39/115/115	-
23	CHL	A2	608	-	-	14/35/111/117	-
23	CHL	7	306	1	-	5/17/93/117	-
24	CLA	c	506	-	-	13/39/115/115	-
25	LUT	BV	615	-	-	1/29/67/67	0/2/2/2
26	NEX	9	617	-	-	17/27/83/83	0/3/3/3
27	LHG	2	406	-	-	18/53/53/53	-
24	CLA	BF	506	-	-	14/39/115/115	-
24	CLA	c	505	-	-	10/39/115/115	-
24	CLA	b	615	-	-	18/39/115/115	-
24	CLA	8	301	3	-	5/9/81/115	-
26	NEX	s	616	-	-	15/27/83/83	0/3/3/3
23	CHL	y	309	-	-	14/35/111/117	-
34	DGD	BD	413	-	-	26/49/89/95	0/2/2/2
23	CHL	7	307	1	-	6/17/93/117	-
27	LHG	L	102	-	-	19/53/53/53	-
24	CLA	0	610	2	-	11/33/109/115	-
24	CLA	BE	605	4	-	19/39/115/115	-
27	LHG	BG	404	-	-	18/53/53/53	-
27	LHG	BY	201	-	-	16/53/53/53	-
38	PHO	R	407	-	-	7/37/103/103	0/5/6/6
24	CLA	c	514	21	-	16/39/115/115	-
29	BCR	v	618	-	-	7/29/63/63	0/2/2/2
24	CLA	v	601	-	-	15/39/115/115	-
24	CLA	1	507	-	-	18/39/115/115	-
29	BCR	Av	101	-	-	4/29/63/63	0/2/2/2
24	CLA	BV	613	14	-	8/20/96/115	-
32	SQD	d	406	-	-	21/45/65/69	0/1/1/1
23	CHL	BU	605	22	-	22/35/111/117	-
23	CHL	A2	609	8	-	11/35/111/117	-
26	NEX	Y	318	-	-	12/27/83/83	0/3/3/3
27	LHG	B	622	-	-	16/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	A	412	-	-	16/43/63/70	0/1/1/1
27	LHG	Az	102	-	-	19/53/53/53	-
24	CLA	y	305	-	-	10/21/97/115	-
29	BCR	Ay	102	-	-	6/29/63/63	0/2/2/2
23	CHL	g	607	-	-	18/35/111/117	-
24	CLA	G	610	8	-	21/38/114/115	-
27	LHG	N	618	24	-	16/53/53/53	-
24	CLA	0	613	-	-	13/31/107/115	-
24	CLA	BB	314	8	-	13/39/115/115	-
24	CLA	BJ	611	27	-	11/33/109/115	-
23	CHL	N	606	8	-	10/22/98/117	-
24	CLA	v	613	4	-	14/39/115/115	-
24	CLA	A6	613	14	-	9/20/96/115	-
32	SQD	a	412	-	-	28/49/69/69	0/1/1/1
28	XAT	AA	318	-	-	12/31/93/93	0/4/4/4
24	CLA	BJ	604	-	-	9/21/97/115	-
23	CHL	r	613	22	-	2/12/88/117	-
24	CLA	9	610	1	-	8/29/105/115	-
27	LHG	6	617	24	-	13/51/51/53	-
24	CLA	d	402	-	-	13/39/115/115	-
30	LMG	C	519	-	-	22/46/66/70	0/1/1/1
24	CLA	v	615	-	-	19/39/115/115	-
24	CLA	BD	406	-	-	8/39/115/115	-
24	CLA	B	613	4	-	13/39/115/115	-
23	CHL	r	606	-	-	6/26/102/117	-
29	BCR	C	515	-	-	5/29/63/63	0/2/2/2
24	CLA	9	612	-	-	8/15/91/115	-
24	CLA	BU	612	22	-	0/4/72/115	-
24	CLA	0	611	27	-	14/27/103/115	-
23	CHL	Y	306	8	-	7/20/96/117	-
24	CLA	BF	511	21	-	15/39/115/115	-
24	CLA	y	304	-	-	9/39/115/115	-
24	CLA	Au	602	8	-	13/39/115/115	-
24	CLA	BQ	611	27	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	s	601	-	-	6/17/93/117	-
24	CLA	Au	604	-	-	6/21/97/115	-
24	CLA	BQ	604	-	-	9/21/97/115	-
27	LHG	G	618	24	-	17/53/53/53	-
32	SQD	Az	101	-	-	18/37/57/69	0/1/1/1
23	CHL	y	310	-	-	20/35/111/117	-
24	CLA	8	303	-	-	7/15/91/115	-
24	CLA	BF	513	-	-	15/39/115/115	-
23	CHL	S	601	14	-	5/17/93/117	-
23	CHL	BV	607	-	-	10/17/93/117	-
23	CHL	BQ	605	8	-	7/20/96/117	-
23	CHL	8	307	3	-	8/17/93/117	-
23	CHL	BU	606	-	-	6/26/102/117	-
23	CHL	Ba	308	-	-	20/35/111/117	-
24	CLA	A2	612	-	-	6/33/109/115	-
23	CHL	6	605	2	-	5/17/93/117	-
24	CLA	C	509	21	-	8/39/115/115	-
24	CLA	7	312	-	-	11/15/91/115	-
26	NEX	r	617	-	-	17/27/83/83	0/3/3/3
24	CLA	BE	609	4	-	13/39/115/115	-
24	CLA	BG	402	-	-	12/39/115/115	-
29	BCR	BD	411	-	-	5/29/63/63	0/2/2/2
34	DGD	BF	518	-	-	21/51/91/95	0/2/2/2
24	CLA	Ba	313	-	-	12/33/109/115	-
29	BCR	F	101	-	-	8/29/63/63	0/2/2/2
24	CLA	n	604	-	-	10/21/97/115	-
26	NEX	n	617	-	-	15/27/83/83	0/3/3/3
27	LHG	Y	319	-	-	20/53/53/53	-
24	CLA	AA	303	1	-	6/35/111/115	-
26	NEX	N	617	-	-	15/27/83/83	0/3/3/3
24	CLA	Au	610	8	-	21/38/114/115	-
24	CLA	N	614	-	-	8/19/95/115	-
24	CLA	s	611	-	-	4/20/96/115	-
28	XAT	5	619	-	-	15/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	N	608	-	-	14/35/111/117	-
27	LHG	0	617	24	-	12/51/51/53	-
24	CLA	v	606	-	-	17/39/115/115	-
28	XAT	9	619	-	-	16/31/93/93	0/4/4/4
25	LUT	BV	614	-	-	2/29/67/67	0/2/2/2
24	CLA	r	602	22	-	8/27/105/115	-
23	CHL	5	605	1	-	7/17/93/117	-
24	CLA	5	603	1	-	12/27/103/115	-
29	BCR	z	101	-	-	3/29/63/63	0/2/2/2
24	CLA	g	611	27	-	11/33/109/115	-
24	CLA	C	507	-	-	16/39/115/115	-
24	CLA	A2	602	8	-	15/39/115/115	-
27	LHG	D	404	-	-	16/53/53/53	-
29	BCR	z	102	-	-	7/29/63/63	0/2/2/2
23	CHL	0	601	2	-	15/33/109/117	-
24	CLA	C	502	21	-	16/39/115/115	-
23	CHL	Y	307	-	-	9/22/98/117	-
25	LUT	BQ	616	-	-	1/29/67/67	0/2/2/2
24	CLA	S	612	14	-	10/27/103/115	-
38	PHO	A	408	-	-	7/37/103/103	0/5/6/6
29	BCR	v	622	-	-	13/29/63/63	0/2/2/2
28	XAT	BB	301	-	-	17/31/93/93	0/4/4/4
24	CLA	BE	612	4	-	11/39/115/115	-
29	BCR	BE	619	-	-	7/29/63/63	0/2/2/2
24	CLA	v	610	-	-	15/39/115/115	-
24	CLA	b	610	-	-	12/39/115/115	-
24	CLA	AA	311	1	-	6/15/93/115	-
23	CHL	0	608	2	-	7/17/93/117	-
30	LMG	B	620	-	-	18/46/66/70	0/1/1/1
23	CHL	G	609	-	-	8/23/101/117	-
24	CLA	s	603	14	-	6/15/91/115	-
24	CLA	7	303	1	-	8/35/111/115	-
24	CLA	G	612	-	-	11/33/109/115	-
24	CLA	G	611	27	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AA	304	-	-	12/27/103/115	-
24	CLA	s	602	14	-	12/35/111/115	-
24	CLA	G	604	-	-	6/21/97/115	-
24	CLA	Ba	315	-	-	6/19/95/115	-
23	CHL	A2	601	8	-	17/35/111/117	-
24	CLA	b	614	-	-	12/39/115/115	-
24	CLA	Y	315	-	-	6/19/95/115	-
32	SQD	BO	102	-	-	21/37/57/69	0/1/1/1
23	CHL	S	605	14	-	11/17/93/117	-
34	DGD	Av	102	-	-	14/51/91/95	0/2/2/2
24	CLA	S	602	14	-	13/35/111/115	-
25	LUT	BJ	615	-	-	2/29/67/67	0/2/2/2
34	DGD	H	102	-	-	14/51/91/95	0/2/2/2
25	LUT	AA	316	-	-	3/29/67/67	0/2/2/2
34	DGD	A	402	-	-	24/48/88/95	0/2/2/2
24	CLA	BD	410	-	-	9/33/109/115	-
24	CLA	d	401	5	-	16/39/115/115	-
24	CLA	1	502	21	-	15/39/115/115	-
28	XAT	BJ	619	-	-	12/31/93/93	0/4/4/4
24	CLA	BV	611	-	-	5/20/96/115	-
29	BCR	B	623	-	-	13/29/63/63	0/2/2/2
24	CLA	C	512	-	-	11/39/115/115	-
27	LHG	b	623	-	-	15/50/50/53	-
30	LMG	Aw	101	-	-	12/35/55/70	0/1/1/1
24	CLA	BB	311	8	-	12/33/109/115	-
23	CHL	7	308	-	-	15/29/105/117	-
24	CLA	v	609	4	-	13/39/115/115	-
24	CLA	b	609	4	-	13/39/115/115	-
30	LMG	B	624	-	-	17/35/55/70	0/1/1/1
24	CLA	9	603	-	-	9/27/103/115	-
28	XAT	BQ	619	-	-	19/31/93/93	0/4/4/4
25	LUT	6	616	-	-	1/29/67/67	0/2/2/2
24	CLA	9	602	1	-	14/35/111/115	-
25	LUT	y	316	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	NEX	A6	616	-	-	13/27/83/83	0/3/3/3
24	CLA	c	509	21	-	16/39/115/115	-
24	CLA	BF	512	21	-	13/39/115/115	-
24	CLA	s	608	-	-	7/15/91/115	-
23	CHL	5	609	-	-	12/31/107/117	-
24	CLA	BF	509	21	-	16/39/115/115	-
28	XAT	AA	301	-	-	11/31/93/93	0/4/4/4
24	CLA	g	602	8	-	15/39/115/115	-
25	LUT	BB	317	-	-	1/29/67/67	0/2/2/2
24	CLA	B	609	-	-	13/39/115/115	-
24	CLA	s	613	14	-	9/20/96/115	-
24	CLA	8	308	-	-	5/15/91/115	-
23	CHL	AB	307	3	-	8/17/93/117	-
29	BCR	H	101	-	-	5/29/63/63	0/2/2/2
23	CHL	6	606	-	-	7/17/93/117	-
24	CLA	c	513	-	-	14/39/115/115	-
24	CLA	N	613	8	-	11/33/109/115	-
24	CLA	y	314	8	-	15/39/115/115	-
24	CLA	6	613	-	-	15/31/107/115	-
25	LUT	Y	317	-	-	1/29/67/67	0/2/2/2
24	CLA	C	504	21	-	14/39/115/115	-
23	CHL	n	601	8	-	19/35/111/117	-
24	CLA	1	512	-	-	11/39/115/115	-
25	LUT	AB	311	-	-	1/29/67/67	0/2/2/2
28	XAT	n	619	-	-	19/31/93/93	0/4/4/4
26	NEX	BQ	617	-	-	16/27/83/83	0/3/3/3
24	CLA	0	612	-	-	8/15/91/115	-
26	NEX	G	617	-	-	19/27/83/83	0/3/3/3
24	CLA	B	606	-	-	17/39/115/115	-
31	PL9	2	404	-	-	5/53/73/73	0/1/1/1
34	DGD	1	518	-	-	20/49/89/95	0/2/2/2
27	LHG	Ba	319	24	-	20/53/53/53	-
24	CLA	N	612	-	-	6/33/109/115	-
23	CHL	BB	308	-	-	15/35/111/117	-
33	HEM	F	102	7	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	BF	520	-	-	27/53/53/53	-
24	CLA	B	612	4	-	13/39/115/115	-
32	SQD	D	406	-	-	21/45/65/69	0/1/1/1
34	DGD	BD	401	-	-	21/48/88/95	0/2/2/2
23	CHL	BJ	605	8	-	7/17/93/117	-
23	CHL	g	606	-	-	6/22/98/117	-
23	CHL	Ba	309	-	-	15/35/111/117	-
24	CLA	6	612	-	-	8/15/91/115	-
24	CLA	9	613	1	-	9/27/103/115	-
26	NEX	BB	320	-	-	17/27/83/83	0/3/3/3
27	LHG	C	521	-	-	23/53/53/53	-
23	CHL	Ba	310	-	-	19/35/111/117	-
34	DGD	BF	517	-	-	14/44/84/95	0/2/2/2
27	LHG	d	404	-	-	16/53/53/53	-
26	NEX	y	318	-	-	13/27/83/83	0/3/3/3
24	CLA	BU	602	22	-	8/27/105/115	-
32	SQD	R	411	-	-	26/49/69/69	0/1/1/1
23	CHL	BQ	608	-	-	13/35/111/117	-
23	CHL	BV	606	-	-	8/26/102/117	-
24	CLA	BV	602	14	-	9/35/111/115	-
30	LMG	BF	501	-	-	22/46/66/70	0/1/1/1
25	LUT	g	615	-	-	2/29/67/67	0/2/2/2
24	CLA	n	611	27	-	14/33/109/115	-
24	CLA	BQ	603	8	-	14/39/115/115	-
24	CLA	BB	315	-	-	6/19/95/115	-
24	CLA	c	511	21	-	15/39/115/115	-
23	CHL	0	609	-	-	9/29/105/117	-
25	LUT	AA	317	-	-	1/29/67/67	0/2/2/2
32	SQD	L	103	-	-	18/49/69/69	0/1/1/1
23	CHL	Au	607	-	-	15/35/111/117	-
24	CLA	BQ	614	-	-	7/19/95/115	-
23	CHL	BV	601	-	-	6/17/93/117	-
24	CLA	9	611	27	-	8/15/91/115	-
24	CLA	BU	611	22	-	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	2	403	-	-	12/39/115/115	-
34	DGD	a	413	-	-	26/49/89/95	0/2/2/2
23	CHL	A6	607	14	-	14/17/93/117	-
23	CHL	y	306	8	-	7/20/96/117	-
24	CLA	1	513	21	-	15/39/115/115	-
23	CHL	A2	607	-	-	16/35/111/117	-
29	BCR	BE	620	-	-	5/29/63/63	0/2/2/2
30	LMG	D	405	-	-	13/41/61/70	0/1/1/1
24	CLA	b	611	-	-	13/39/115/115	-
24	CLA	A	405	20	-	10/39/115/115	-
24	CLA	AA	313	-	-	4/15/91/115	-
28	XAT	7	301	-	-	11/31/93/93	0/4/4/4
24	CLA	C	506	21	-	17/39/115/115	-
24	CLA	g	612	-	-	6/33/109/115	-
23	CHL	BB	302	8	-	16/35/111/117	-
24	CLA	S	604	-	-	9/21/97/115	-
24	CLA	n	614	-	-	7/19/95/115	-
24	CLA	9	604	-	-	12/21/97/115	-
24	CLA	A6	602	14	-	13/35/111/115	-
24	CLA	n	603	8	-	16/39/115/115	-
23	CHL	N	601	8	-	17/35/111/117	-
23	CHL	AA	308	-	-	17/29/105/117	-
24	CLA	AA	312	-	-	11/15/91/115	-
34	DGD	1	516	-	-	12/44/84/95	0/2/2/2
26	NEX	g	617	-	-	17/27/83/83	0/3/3/3
27	LHG	c	519	-	-	26/53/53/53	-
24	CLA	2	402	5	-	17/39/115/115	-
24	CLA	Y	303	8	-	22/39/115/115	-
24	CLA	r	610	27	-	11/20/96/115	-
23	CHL	BB	309	-	-	14/35/111/117	-
25	LUT	7	317	-	-	1/29/67/67	0/2/2/2
26	NEX	S	616	-	-	15/27/83/83	0/3/3/3
25	LUT	7	316	-	-	3/29/67/67	0/2/2/2
24	CLA	r	612	22	-	0/4/72/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	6	609	-	-	10/29/105/117	-
38	PHO	R	408	-	-	15/37/103/103	0/5/6/6
25	LUT	n	616	-	-	1/29/67/67	0/2/2/2
24	CLA	v	607	-	-	20/39/115/115	-
28	XAT	Au	619	-	-	14/31/93/93	0/4/4/4
24	CLA	Au	603	8	-	14/39/115/115	-
27	LHG	y	319	24	-	20/53/53/53	-
24	CLA	C	513	21	-	14/39/115/115	-
27	LHG	r	618	24	-	12/46/46/53	-
23	CHL	S	607	-	-	11/17/93/117	-
24	CLA	s	609	14	-	8/27/103/115	-
29	BCR	1	515	-	-	5/29/63/63	0/2/2/2
24	CLA	A2	611	27	-	15/33/109/115	-
24	CLA	C	503	21	-	16/39/115/115	-
25	LUT	BB	316	-	-	3/29/67/67	0/2/2/2
23	CHL	AB	304	3	-	10/17/93/117	-
23	CHL	G	601	8	-	16/35/111/117	-
24	CLA	6	614	2	-	12/19/95/115	-
24	CLA	b	604	4	-	13/39/115/115	-
27	LHG	1	521	-	-	23/53/53/53	-
30	LMG	i	101	-	-	17/43/63/70	0/1/1/1
29	BCR	Bb	101	-	-	7/29/63/63	0/2/2/2
32	SQD	A	413	-	-	26/49/69/69	0/1/1/1
29	BCR	B	617	-	-	5/29/63/63	0/2/2/2
24	CLA	c	508	-	-	14/39/115/115	-
25	LUT	8	311	-	-	1/29/67/67	0/2/2/2
26	NEX	BJ	617	-	-	17/27/83/83	0/3/3/3
24	CLA	0	604	-	-	8/15/91/115	-
32	SQD	BG	406	-	-	23/45/65/69	0/1/1/1
23	CHL	n	607	-	-	16/35/111/117	-
23	CHL	y	307	-	-	7/22/98/117	-
24	CLA	Ba	304	-	-	9/39/115/115	-
23	CHL	5	608	-	-	7/17/93/117	-
30	LMG	c	501	-	-	23/46/66/70	0/1/1/1
25	LUT	s	615	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	Ay	101	-	-	11/29/63/63	0/2/2/2
23	CHL	9	607	-	-	18/32/108/117	-
24	CLA	A	407	-	-	7/21/97/115	-
24	CLA	r	609	22	-	12/39/115/115	-
23	CHL	9	608	-	-	7/17/93/117	-
23	CHL	s	607	-	-	9/17/93/117	-
24	CLA	6	604	-	-	10/15/91/115	-
24	CLA	BU	610	27	-	10/20/96/115	-
24	CLA	n	602	8	-	16/39/115/115	-
25	LUT	Ba	316	-	-	2/29/67/67	0/2/2/2
27	LHG	1	520	-	-	25/53/53/53	-
29	BCR	b	601	-	-	15/29/63/63	0/2/2/2
24	CLA	BF	514	-	-	15/39/115/115	-
24	CLA	BE	611	-	-	14/39/115/115	-
24	CLA	R	406	-	-	7/21/97/115	-
29	BCR	v	617	-	-	5/29/63/63	0/2/2/2
24	CLA	Y	312	-	-	13/33/109/115	-
24	CLA	b	606	4	-	17/39/115/115	-
24	CLA	A2	604	-	-	9/21/97/115	-
24	CLA	BE	604	4	-	13/39/115/115	-
23	CHL	AB	306	-	-	5/17/93/117	-
24	CLA	BJ	610	8	-	21/38/114/115	-
28	XAT	G	619	-	-	14/31/93/93	0/4/4/4
29	BCR	b	619	-	-	7/29/63/63	0/2/2/2
34	DGD	R	401	-	-	24/48/88/95	0/2/2/2
24	CLA	y	303	8	-	16/39/115/115	-
24	CLA	s	612	14	-	10/27/103/115	-
23	CHL	Y	302	8	-	15/35/111/117	-
30	LMG	b	621	-	-	25/46/66/70	0/1/1/1
23	CHL	BB	310	-	-	17/35/111/117	-
27	LHG	5	618	24	-	18/45/45/53	-
23	CHL	Ba	302	8	-	14/35/111/117	-
24	CLA	BB	305	-	-	11/21/97/115	-
24	CLA	A6	603	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	s	614	-	-	2/29/67/67	0/2/2/2
25	LUT	G	615	-	-	1/29/67/67	0/2/2/2
24	CLA	8	310	-	-	4/15/91/115	-
23	CHL	A6	606	-	-	7/26/102/117	-
24	CLA	n	613	-	-	11/33/109/115	-
24	CLA	BE	614	-	-	12/39/115/115	-
23	CHL	BB	307	-	-	8/22/98/117	-
24	CLA	G	603	8	-	14/39/115/115	-
28	XAT	g	619	-	-	12/31/93/93	0/4/4/4
24	CLA	5	604	-	-	12/21/97/115	-
31	PL9	D	403	-	-	5/53/73/73	0/1/1/1
24	CLA	BE	606	4	-	18/39/115/115	-
23	CHL	BJ	606	-	-	6/22/98/117	-
27	LHG	b	622	-	-	24/53/53/53	-
33	HEM	4	102	7	-	6/14/54/54	-
24	CLA	BQ	613	-	-	11/33/109/115	-
24	CLA	Ba	314	8	-	15/39/115/115	-
24	CLA	1	504	21	-	14/39/115/115	-
23	CHL	g	605	8	-	7/17/93/117	-
24	CLA	g	603	8	-	13/39/115/115	-
27	LHG	BE	623	-	-	15/50/50/53	-
30	LMG	BE	621	-	-	23/46/66/70	0/1/1/1
24	CLA	6	610	2	-	10/33/109/115	-
24	CLA	a	410	-	-	9/33/109/115	-
23	CHL	AA	310	-	-	12/29/105/117	-
24	CLA	b	607	-	-	14/39/115/115	-
29	BCR	A	411	-	-	5/29/63/63	0/2/2/2
24	CLA	a	406	-	-	7/39/115/115	-
23	CHL	s	605	14	-	11/17/93/117	-
24	CLA	5	610	1	-	8/29/105/115	-
32	SQD	l	101	-	-	21/49/69/69	0/1/1/1
24	CLA	b	608	-	-	19/39/115/115	-
25	LUT	A6	615	-	-	1/29/67/67	0/2/2/2
34	DGD	c	516	-	-	14/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	1	505	-	-	9/39/115/115	-
25	LUT	Au	615	-	-	1/29/67/67	0/2/2/2
24	CLA	r	603	22	-	7/33/109/115	-
24	CLA	BE	610	-	-	14/39/115/115	-
25	LUT	A2	615	-	-	1/29/67/67	0/2/2/2
27	LHG	BE	622	-	-	24/53/53/53	-
24	CLA	B	605	4	-	22/39/115/115	-
24	CLA	BB	313	-	-	11/33/109/115	-
23	CHL	Au	606	-	-	9/22/98/117	-
24	CLA	r	608	22	-	13/31/107/115	-
23	CHL	BQ	606	8	-	11/22/98/117	-
38	PHO	BD	408	-	-	7/37/103/103	0/5/6/6
23	CHL	A2	606	8	-	10/22/98/117	-
23	CHL	r	607	22	-	19/29/105/117	-
23	CHL	Ba	306	8	-	7/20/96/117	-
24	CLA	BV	609	14	-	9/27/103/115	-
24	CLA	AA	305	-	-	7/15/91/115	-
24	CLA	B	607	-	-	20/39/115/115	-
24	CLA	c	510	21	-	8/39/115/115	-
24	CLA	B	615	-	-	19/39/115/115	-
24	CLA	6	611	27	-	14/27/103/115	-
24	CLA	A6	608	-	-	6/15/91/115	-
24	CLA	BJ	603	8	-	13/39/115/115	-
24	CLA	1	503	21	-	13/39/115/115	-
25	LUT	9	615	-	-	3/29/67/67	0/2/2/2
23	CHL	n	606	8	-	11/22/98/117	-
23	CHL	BQ	601	8	-	18/35/111/117	-
24	CLA	N	611	27	-	15/33/109/115	-
25	LUT	BU	615	-	-	3/29/67/67	0/2/2/2
30	LMG	v	620	-	-	18/46/66/70	0/1/1/1
32	SQD	l	102	-	-	21/37/57/69	0/1/1/1
29	BCR	h	101	-	-	5/29/63/63	0/2/2/2
23	CHL	9	605	1	-	7/17/93/117	-
24	CLA	G	602	8	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	1	506	21	-	17/39/115/115	-
24	CLA	BF	505	-	-	8/39/115/115	-
24	CLA	B	611	4	-	11/39/115/115	-
24	CLA	v	603	4	-	13/39/115/115	-
24	CLA	BF	510	21	-	8/39/115/115	-
27	LHG	2	405	-	-	15/50/50/53	-
31	PL9	d	403	-	-	10/53/73/73	0/1/1/1
23	CHL	BV	605	14	-	10/17/93/117	-
24	CLA	B	604	4	-	14/39/115/115	-
28	XAT	r	616	-	-	17/31/93/93	0/4/4/4
24	CLA	v	611	4	-	11/39/115/115	-
23	CHL	BU	607	22	-	18/29/105/117	-
23	CHL	6	601	2	-	16/33/109/117	-
25	LUT	A6	614	-	-	2/29/67/67	0/2/2/2
26	NEX	A2	617	-	-	15/27/83/83	0/3/3/3
24	CLA	BV	612	14	-	10/27/103/115	-
24	CLA	Y	304	8	-	11/39/115/115	-
26	NEX	Au	617	-	-	19/27/83/83	0/3/3/3
29	BCR	K	102	-	-	6/29/63/63	0/2/2/2
24	CLA	BU	609	22	-	12/39/115/115	-
23	CHL	7	310	-	-	14/29/105/117	-
24	CLA	AB	308	-	-	6/15/91/115	-
28	XAT	A2	619	-	-	17/31/93/93	0/4/4/4
24	CLA	BG	401	5	-	16/39/115/115	-
34	DGD	C	518	-	-	20/49/89/95	0/2/2/2
25	LUT	BJ	616	-	-	1/29/67/67	0/2/2/2
29	BCR	a	411	-	-	5/29/63/63	0/2/2/2
24	CLA	A2	603	8	-	13/39/115/115	-
23	CHL	G	607	-	-	15/35/111/117	-
29	BCR	BF	516	-	-	6/29/63/63	0/2/2/2
24	CLA	6	603	-	-	9/27/103/115	-
23	CHL	Y	308	-	-	15/35/111/117	-
23	CHL	BQ	609	-	-	15/35/111/117	-
24	CLA	7	311	1	-	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	2	407	-	-	13/41/61/70	0/1/1/1
23	CHL	5	601	1	-	9/17/93/117	-
24	CLA	1	509	21	-	8/39/115/115	-
24	CLA	B	614	-	-	19/39/115/115	-
25	LUT	9	616	-	-	1/29/67/67	0/2/2/2
29	BCR	k	101	-	-	11/29/63/63	0/2/2/2
32	SQD	L	101	-	-	19/37/57/69	0/1/1/1
24	CLA	7	314	1	-	7/15/91/115	-
24	CLA	BE	616	-	-	12/39/115/115	-
28	XAT	y	301	-	-	15/31/93/93	0/4/4/4
24	CLA	BE	607	-	-	14/39/115/115	-
25	LUT	g	616	-	-	1/29/67/67	0/2/2/2
24	CLA	N	604	-	-	9/21/97/115	-
25	LUT	0	615	-	-	2/29/67/67	0/2/2/2
24	CLA	BJ	614	8	-	5/19/95/115	-
24	CLA	BB	304	8	-	11/39/115/115	-
29	BCR	BK	101	-	-	6/29/63/63	0/2/2/2
23	CHL	Ba	307	-	-	8/22/98/117	-
23	CHL	N	609	8	-	12/35/111/117	-
24	CLA	A6	610	-	-	10/29/105/115	-
29	BCR	b	620	-	-	4/29/63/63	0/2/2/2
24	CLA	G	613	-	-	12/39/115/115	-
30	LMG	BG	405	-	-	14/41/61/70	0/1/1/1
24	CLA	v	612	4	-	13/39/115/115	-
24	CLA	A6	612	14	-	11/27/103/115	-
27	LHG	BB	319	-	-	18/53/53/53	-
24	CLA	r	611	22	-	6/20/96/115	-
27	LHG	BU	617	24	-	12/46/46/53	-
27	LHG	W	201	-	-	15/53/53/53	-
34	DGD	BK	102	-	-	18/51/91/95	0/2/2/2
34	DGD	1	517	-	-	21/51/91/95	0/2/2/2
24	CLA	0	602	2	-	16/33/109/115	-
24	CLA	c	502	21	-	14/39/115/115	-
24	CLA	7	305	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	303	-	-	7/15/91/115	-
24	CLA	A6	611	-	-	6/20/96/115	-
24	CLA	BF	502	21	-	14/39/115/115	-
24	CLA	g	613	-	-	13/39/115/115	-
28	XAT	7	318	-	-	12/31/93/93	0/4/4/4
23	CHL	BJ	609	-	-	10/29/105/117	-
29	BCR	K	101	-	-	11/29/63/63	0/2/2/2
25	LUT	BQ	615	-	-	1/29/67/67	0/2/2/2
34	DGD	C	516	-	-	13/44/84/95	0/2/2/2
29	BCR	BE	601	-	-	15/29/63/63	0/2/2/2
23	CHL	6	607	-	-	12/26/102/117	-
24	CLA	b	605	4	-	19/39/115/115	-
29	BCR	v	619	-	-	7/29/63/63	0/2/2/2
23	CHL	A6	605	14	-	11/17/93/117	-

All (7506) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	7	301	XAT	C10-C9	15.13	1.55	1.35
28	AA	301	XAT	C10-C9	15.11	1.55	1.35
28	Au	619	XAT	C10-C9	15.10	1.55	1.35
28	G	619	XAT	C10-C9	15.07	1.55	1.35
28	AA	318	XAT	C10-C9	15.04	1.55	1.35
28	BJ	619	XAT	C10-C9	15.04	1.55	1.35
28	g	619	XAT	C10-C9	15.04	1.55	1.35
28	9	619	XAT	C14-C13	15.03	1.55	1.35
28	8	312	XAT	C10-C9	15.03	1.55	1.35
28	AB	312	XAT	C10-C9	14.99	1.55	1.35
28	7	318	XAT	C10-C9	14.98	1.55	1.35
28	g	619	XAT	C14-C13	14.95	1.55	1.35
28	y	301	XAT	C10-C9	14.95	1.55	1.35
28	7	301	XAT	C14-C13	14.94	1.55	1.35
28	BJ	619	XAT	C14-C13	14.94	1.55	1.35
28	BB	301	XAT	C10-C9	14.93	1.55	1.35
28	Ba	301	XAT	C10-C9	14.92	1.55	1.35
28	AA	301	XAT	C14-C13	14.91	1.55	1.35
28	BQ	619	XAT	C10-C9	14.88	1.55	1.35
28	BB	301	XAT	C14-C13	14.87	1.55	1.35
28	AA	301	XAT	C30-C29	14.87	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	619	XAT	C30-C29	14.86	1.55	1.35
28	n	619	XAT	C10-C9	14.85	1.55	1.35
28	Y	301	XAT	C10-C9	14.85	1.55	1.35
28	7	301	XAT	C30-C29	14.84	1.55	1.35
28	Y	301	XAT	C14-C13	14.84	1.55	1.35
28	G	619	XAT	C14-C13	14.82	1.55	1.35
28	Au	619	XAT	C30-C29	14.82	1.55	1.35
28	Au	619	XAT	C14-C13	14.81	1.55	1.35
28	Y	301	XAT	C30-C29	14.79	1.55	1.35
28	BB	301	XAT	C30-C29	14.79	1.55	1.35
28	7	318	XAT	C14-C13	14.76	1.55	1.35
28	Ba	301	XAT	C30-C29	14.75	1.55	1.35
28	5	619	XAT	C14-C13	14.75	1.55	1.35
28	AA	318	XAT	C14-C13	14.75	1.55	1.35
28	BQ	619	XAT	C14-C13	14.74	1.55	1.35
28	g	619	XAT	C30-C29	14.72	1.55	1.35
28	BQ	619	XAT	C30-C29	14.71	1.55	1.35
28	n	619	XAT	C14-C13	14.70	1.55	1.35
28	N	619	XAT	C30-C29	14.70	1.55	1.35
28	BJ	619	XAT	C30-C29	14.69	1.55	1.35
28	N	619	XAT	C14-C13	14.69	1.55	1.35
28	y	301	XAT	C14-C13	14.67	1.55	1.35
28	n	619	XAT	C30-C29	14.66	1.55	1.35
28	A2	619	XAT	C14-C13	14.66	1.55	1.35
28	A2	619	XAT	C30-C29	14.66	1.55	1.35
28	8	312	XAT	C30-C29	14.65	1.55	1.35
28	y	301	XAT	C30-C29	14.65	1.55	1.35
28	Ba	301	XAT	C14-C13	14.65	1.55	1.35
28	r	616	XAT	C10-C9	14.62	1.55	1.35
28	N	619	XAT	C10-C9	14.62	1.55	1.35
28	5	619	XAT	C10-C9	14.61	1.55	1.35
28	AB	312	XAT	C30-C29	14.60	1.55	1.35
28	9	619	XAT	C10-C9	14.59	1.55	1.35
28	BU	616	XAT	C10-C9	14.59	1.55	1.35
28	7	318	XAT	C30-C29	14.58	1.55	1.35
28	BB	301	XAT	C34-C33	14.57	1.55	1.35
28	BU	616	XAT	C14-C13	14.55	1.55	1.35
28	Y	301	XAT	C34-C33	14.55	1.55	1.35
28	A2	619	XAT	C10-C9	14.55	1.55	1.35
28	Au	619	XAT	C34-C33	14.53	1.55	1.35
28	7	301	XAT	C34-C33	14.51	1.55	1.35
28	AA	318	XAT	C30-C29	14.49	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	r	616	XAT	C14-C13	14.47	1.55	1.35
28	G	619	XAT	C34-C33	14.47	1.55	1.35
28	g	619	XAT	C34-C33	14.45	1.54	1.35
28	AA	301	XAT	C34-C33	14.45	1.54	1.35
28	7	318	XAT	C34-C33	14.45	1.54	1.35
28	9	619	XAT	C34-C33	14.42	1.54	1.35
28	BJ	619	XAT	C34-C33	14.42	1.54	1.35
28	8	312	XAT	C34-C33	14.42	1.54	1.35
28	r	616	XAT	C34-C33	14.42	1.54	1.35
28	n	619	XAT	C34-C33	14.41	1.54	1.35
28	9	619	XAT	C30-C29	14.39	1.54	1.35
28	y	301	XAT	C34-C33	14.38	1.54	1.35
28	8	312	XAT	C14-C13	14.38	1.54	1.35
28	AA	318	XAT	C34-C33	14.38	1.54	1.35
28	Ba	301	XAT	C34-C33	14.38	1.54	1.35
28	BQ	619	XAT	C34-C33	14.37	1.54	1.35
28	r	616	XAT	C30-C29	14.36	1.54	1.35
28	5	619	XAT	C30-C29	14.36	1.54	1.35
28	AB	312	XAT	C34-C33	14.36	1.54	1.35
28	AB	312	XAT	C14-C13	14.35	1.54	1.35
28	N	619	XAT	C34-C33	14.33	1.54	1.35
28	BU	616	XAT	C30-C29	14.30	1.54	1.35
28	BU	616	XAT	C34-C33	14.29	1.54	1.35
28	A2	619	XAT	C34-C33	14.25	1.54	1.35
28	5	619	XAT	C34-C33	14.15	1.54	1.35
28	A2	619	XAT	C8-C7	11.07	1.56	1.32
28	7	301	XAT	C8-C7	11.06	1.56	1.32
28	AA	301	XAT	C8-C7	11.06	1.56	1.32
28	g	619	XAT	C8-C7	11.04	1.56	1.32
28	N	619	XAT	C8-C7	11.03	1.56	1.32
28	BJ	619	XAT	C8-C7	11.02	1.56	1.32
28	Au	619	XAT	C8-C7	10.98	1.56	1.32
28	8	312	XAT	C8-C7	10.97	1.56	1.32
28	7	318	XAT	C8-C7	10.96	1.56	1.32
28	G	619	XAT	C8-C7	10.95	1.56	1.32
28	AB	312	XAT	C8-C7	10.95	1.56	1.32
28	Y	301	XAT	C8-C7	10.94	1.56	1.32
28	AA	318	XAT	C8-C7	10.93	1.56	1.32
28	BB	301	XAT	C8-C7	10.93	1.56	1.32
28	Ba	301	XAT	C8-C7	10.91	1.56	1.32
28	n	619	XAT	C8-C7	10.88	1.56	1.32
28	y	301	XAT	C8-C7	10.87	1.56	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BQ	619	XAT	C8-C7	10.86	1.56	1.32
28	r	616	XAT	C8-C7	10.83	1.56	1.32
28	BU	616	XAT	C8-C7	10.81	1.56	1.32
28	BJ	619	XAT	C28-C27	10.78	1.56	1.32
28	g	619	XAT	C28-C27	10.77	1.56	1.32
28	9	619	XAT	C8-C7	10.77	1.56	1.32
28	BU	616	XAT	C28-C27	10.74	1.56	1.32
28	r	616	XAT	C28-C27	10.73	1.55	1.32
28	BQ	619	XAT	C28-C27	10.73	1.55	1.32
28	G	619	XAT	C28-C27	10.73	1.55	1.32
28	Y	301	XAT	C28-C27	10.72	1.55	1.32
28	7	301	XAT	C28-C27	10.71	1.55	1.32
28	BB	301	XAT	C28-C27	10.71	1.55	1.32
28	Au	619	XAT	C28-C27	10.71	1.55	1.32
28	5	619	XAT	C8-C7	10.70	1.55	1.32
28	n	619	XAT	C28-C27	10.70	1.55	1.32
28	9	619	XAT	C28-C27	10.68	1.55	1.32
28	5	619	XAT	C28-C27	10.68	1.55	1.32
28	AA	301	XAT	C28-C27	10.67	1.55	1.32
28	A2	619	XAT	C28-C27	10.67	1.55	1.32
28	y	301	XAT	C28-C27	10.67	1.55	1.32
28	Ba	301	XAT	C28-C27	10.66	1.55	1.32
28	N	619	XAT	C28-C27	10.65	1.55	1.32
28	7	318	XAT	C28-C27	10.59	1.55	1.32
28	AA	318	XAT	C28-C27	10.58	1.55	1.32
28	8	312	XAT	C28-C27	10.58	1.55	1.32
28	AB	312	XAT	C28-C27	10.55	1.55	1.32
38	a	409	PHO	C1B-C2B	9.29	1.49	1.39
38	BD	409	PHO	C1B-C2B	9.25	1.49	1.39
38	a	408	PHO	C1B-C2B	8.93	1.49	1.39
38	A	409	PHO	C1B-C2B	8.92	1.49	1.39
38	R	408	PHO	C1B-C2B	8.86	1.49	1.39
38	BD	408	PHO	C1B-C2B	8.80	1.49	1.39
38	A	408	PHO	C1B-C2B	8.72	1.49	1.39
38	R	407	PHO	C1B-C2B	8.67	1.49	1.39
28	AA	301	XAT	C31-C32	8.11	1.55	1.34
28	7	301	XAT	C11-C12	8.09	1.55	1.34
28	7	301	XAT	C31-C32	8.09	1.55	1.34
28	AA	301	XAT	C11-C12	8.09	1.55	1.34
28	g	619	XAT	C11-C12	8.05	1.55	1.34
28	A2	619	XAT	C11-C12	8.04	1.55	1.34
28	BB	301	XAT	C11-C12	8.03	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	301	XAT	C11-C12	8.03	1.55	1.34
28	BJ	619	XAT	C11-C12	8.02	1.55	1.34
28	BQ	619	XAT	C11-C12	8.01	1.55	1.34
28	A2	619	XAT	C31-C32	8.01	1.55	1.34
28	Au	619	XAT	C11-C12	8.01	1.55	1.34
28	Au	619	XAT	C31-C32	8.01	1.55	1.34
28	G	619	XAT	C31-C32	8.00	1.55	1.34
28	7	318	XAT	C11-C12	8.00	1.55	1.34
28	N	619	XAT	C11-C12	8.00	1.55	1.34
28	AB	312	XAT	C31-C32	8.00	1.55	1.34
28	BB	301	XAT	C31-C32	7.99	1.55	1.34
28	G	619	XAT	C11-C12	7.99	1.55	1.34
28	8	312	XAT	C11-C12	7.99	1.55	1.34
28	AA	318	XAT	C11-C12	7.98	1.55	1.34
28	n	619	XAT	C11-C12	7.98	1.55	1.34
28	N	619	XAT	C31-C32	7.98	1.55	1.34
28	8	312	XAT	C31-C32	7.97	1.55	1.34
28	BU	616	XAT	C11-C12	7.97	1.55	1.34
28	Y	301	XAT	C31-C32	7.97	1.55	1.34
28	9	619	XAT	C11-C12	7.96	1.55	1.34
28	r	616	XAT	C11-C12	7.95	1.55	1.34
28	AB	312	XAT	C11-C12	7.95	1.55	1.34
28	Ba	301	XAT	C11-C12	7.94	1.55	1.34
28	AA	318	XAT	C31-C32	7.94	1.55	1.34
28	BJ	619	XAT	C31-C32	7.94	1.55	1.34
28	y	301	XAT	C11-C12	7.93	1.55	1.34
28	g	619	XAT	C31-C32	7.92	1.55	1.34
28	7	318	XAT	C31-C32	7.92	1.55	1.34
28	n	619	XAT	C31-C32	7.91	1.55	1.34
28	BQ	619	XAT	C31-C32	7.90	1.54	1.34
28	5	619	XAT	C11-C12	7.88	1.54	1.34
28	y	301	XAT	C31-C32	7.84	1.54	1.34
28	r	616	XAT	C31-C32	7.83	1.54	1.34
28	BU	616	XAT	C31-C32	7.81	1.54	1.34
28	Ba	301	XAT	C31-C32	7.79	1.54	1.34
28	9	619	XAT	C31-C32	7.75	1.54	1.34
28	5	619	XAT	C31-C32	7.70	1.54	1.34
28	Au	619	XAT	C35-C15	7.46	1.55	1.36
28	G	619	XAT	C35-C15	7.43	1.55	1.36
28	A2	619	XAT	C35-C15	7.40	1.55	1.36
28	7	301	XAT	C35-C15	7.40	1.55	1.36
28	AA	301	XAT	C35-C15	7.38	1.55	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BB	301	XAT	C35-C15	7.37	1.55	1.36
28	N	619	XAT	C35-C15	7.34	1.55	1.36
28	Y	301	XAT	C35-C15	7.33	1.55	1.36
28	BJ	619	XAT	C35-C15	7.30	1.55	1.36
28	BQ	619	XAT	C35-C15	7.29	1.54	1.36
28	g	619	XAT	C35-C15	7.28	1.54	1.36
28	n	619	XAT	C35-C15	7.28	1.54	1.36
28	7	318	XAT	C35-C15	7.27	1.54	1.36
28	9	619	XAT	C35-C15	7.27	1.54	1.36
28	AA	318	XAT	C35-C15	7.27	1.54	1.36
28	y	301	XAT	C35-C15	7.26	1.54	1.36
28	Ba	301	XAT	C35-C15	7.25	1.54	1.36
28	8	312	XAT	C35-C15	7.25	1.54	1.36
28	AB	312	XAT	C35-C15	7.23	1.54	1.36
28	BU	616	XAT	C35-C15	7.22	1.54	1.36
28	r	616	XAT	C35-C15	7.21	1.54	1.36
28	5	619	XAT	C35-C15	7.15	1.54	1.36
38	a	408	PHO	C3B-C4B	7.13	1.49	1.41
38	A	408	PHO	C3B-C4B	7.13	1.49	1.41
38	BD	408	PHO	C3B-C4B	7.12	1.49	1.41
38	R	407	PHO	C3B-C4B	7.09	1.49	1.41
38	a	409	PHO	C3B-C4B	6.96	1.49	1.41
38	BD	409	PHO	C3B-C4B	6.90	1.49	1.41
38	A	409	PHO	C3B-C4B	6.90	1.49	1.41
38	R	408	PHO	C3B-C4B	6.84	1.49	1.41
31	D	403	PL9	C3-C4	-6.82	1.38	1.49
23	y	309	CHL	O2D-CGD	6.20	1.48	1.33
31	2	404	PL9	C3-C4	-5.98	1.39	1.49
23	9	609	CHL	CHC-C1C	5.55	1.49	1.38
31	D	403	PL9	C7-C3	-5.48	1.45	1.51
23	0	609	CHL	CHC-C1C	5.41	1.49	1.38
23	5	609	CHL	CHC-C1C	5.40	1.49	1.38
23	9	609	CHL	C3D-C4D	-5.23	1.32	1.44
23	BQ	605	CHL	O2D-CGD	5.21	1.45	1.33
23	BV	607	CHL	O2D-CGD	5.21	1.45	1.33
23	s	607	CHL	O2D-CGD	5.21	1.45	1.33
23	AA	307	CHL	O2D-CGD	5.20	1.45	1.33
31	2	404	PL9	C7-C3	-5.20	1.46	1.51
23	BV	601	CHL	O2D-CGD	5.19	1.45	1.33
23	g	606	CHL	O2D-CGD	5.18	1.45	1.33
23	6	605	CHL	O2D-CGD	5.18	1.45	1.33
23	n	607	CHL	O2D-CGD	5.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BQ	607	CHL	O2D-CGD	5.18	1.45	1.33
23	g	607	CHL	O2D-CGD	5.17	1.45	1.33
23	BJ	609	CHL	O2D-CGD	5.16	1.45	1.33
23	N	607	CHL	O2D-CGD	5.16	1.45	1.33
23	y	308	CHL	O2D-CGD	5.16	1.45	1.33
23	g	609	CHL	O2D-CGD	5.16	1.45	1.33
23	BJ	606	CHL	O2D-CGD	5.16	1.45	1.33
23	7	306	CHL	O2D-CGD	5.16	1.45	1.33
23	7	307	CHL	O2D-CGD	5.16	1.45	1.33
23	Au	607	CHL	O2D-CGD	5.16	1.45	1.33
23	Ba	308	CHL	O2D-CGD	5.16	1.45	1.33
23	n	605	CHL	O2D-CGD	5.15	1.45	1.33
23	BQ	606	CHL	O2D-CGD	5.15	1.45	1.33
23	BJ	607	CHL	O2D-CGD	5.15	1.45	1.33
23	6	607	CHL	O2D-CGD	5.15	1.45	1.33
23	0	605	CHL	O2D-CGD	5.15	1.45	1.33
23	A2	607	CHL	O2D-CGD	5.15	1.45	1.33
23	AB	305	CHL	O2D-CGD	5.14	1.45	1.33
23	AA	306	CHL	O2D-CGD	5.14	1.45	1.33
23	Ba	309	CHL	O2D-CGD	5.13	1.45	1.33
23	Au	605	CHL	O2D-CGD	5.13	1.45	1.33
23	8	305	CHL	O2D-CGD	5.13	1.45	1.33
23	G	605	CHL	O2D-CGD	5.13	1.45	1.33
23	G	607	CHL	O2D-CGD	5.12	1.45	1.33
23	s	601	CHL	O2D-CGD	5.12	1.45	1.33
23	A2	609	CHL	C3D-C4D	-5.11	1.32	1.44
23	0	607	CHL	O2D-CGD	5.11	1.45	1.33
23	BB	310	CHL	C3D-C4D	-5.11	1.32	1.44
23	AB	307	CHL	C3D-C4D	-5.10	1.32	1.44
23	g	605	CHL	O2D-CGD	5.10	1.45	1.33
23	AA	310	CHL	O2D-CGD	5.10	1.45	1.33
23	BJ	605	CHL	O2D-CGD	5.10	1.45	1.33
23	Ba	310	CHL	O2D-CGD	5.09	1.45	1.33
23	r	606	CHL	O2D-CGD	5.09	1.45	1.33
23	y	307	CHL	O2D-CGD	5.09	1.45	1.33
23	A6	601	CHL	O2D-CGD	5.09	1.45	1.33
23	6	606	CHL	O2D-CGD	5.09	1.45	1.33
23	9	608	CHL	C3D-C4D	-5.09	1.32	1.44
23	BQ	608	CHL	O2D-CGD	5.09	1.45	1.33
23	S	607	CHL	O2D-CGD	5.08	1.45	1.33
23	Ba	307	CHL	O2D-CGD	5.08	1.45	1.33
23	S	601	CHL	O2D-CGD	5.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	310	CHL	O2D-CGD	5.08	1.45	1.33
23	n	606	CHL	O2D-CGD	5.08	1.45	1.33
23	g	601	CHL	O2D-CGD	5.07	1.45	1.33
23	BB	302	CHL	C3D-C4D	-5.07	1.32	1.44
23	9	605	CHL	O2D-CGD	5.07	1.45	1.33
23	n	608	CHL	O2D-CGD	5.07	1.45	1.33
23	BJ	601	CHL	O2D-CGD	5.07	1.45	1.33
23	Y	306	CHL	O2D-CGD	5.07	1.45	1.33
23	BB	306	CHL	O2D-CGD	5.07	1.45	1.33
23	5	609	CHL	C3D-C4D	-5.07	1.32	1.44
23	5	605	CHL	O2D-CGD	5.07	1.45	1.33
23	BQ	601	CHL	O2D-CGD	5.07	1.45	1.33
23	0	609	CHL	C3D-C4D	-5.06	1.32	1.44
23	Y	310	CHL	C3D-C4D	-5.06	1.32	1.44
23	BV	605	CHL	O2D-CGD	5.06	1.45	1.33
23	AA	302	CHL	O2D-CGD	5.06	1.45	1.33
23	BU	613	CHL	C3D-C4D	-5.06	1.32	1.44
23	Y	308	CHL	O2D-CGD	5.05	1.45	1.33
23	6	609	CHL	C3D-C4D	-5.05	1.32	1.44
23	G	606	CHL	O2D-CGD	5.05	1.45	1.33
23	s	605	CHL	O2D-CGD	5.05	1.45	1.33
23	N	601	CHL	O2D-CGD	5.05	1.45	1.33
23	BU	606	CHL	O2D-CGD	5.05	1.45	1.33
23	8	306	CHL	O2D-CGD	5.05	1.45	1.33
23	BQ	609	CHL	O2D-CGD	5.04	1.45	1.33
23	7	308	CHL	O2D-CGD	5.04	1.45	1.33
23	g	609	CHL	CHD-C1D	5.04	1.48	1.38
23	Au	606	CHL	O2D-CGD	5.04	1.45	1.33
23	7	302	CHL	O2D-CGD	5.03	1.45	1.33
23	N	609	CHL	C3D-C4D	-5.03	1.32	1.44
23	n	601	CHL	O2D-CGD	5.03	1.45	1.33
23	9	606	CHL	O2D-CGD	5.03	1.45	1.33
23	AA	308	CHL	O2D-CGD	5.03	1.45	1.33
23	y	306	CHL	O2D-CGD	5.03	1.45	1.33
23	A2	601	CHL	O2D-CGD	5.03	1.45	1.33
23	BB	308	CHL	O2D-CGD	5.03	1.45	1.33
23	BJ	608	CHL	O2D-CGD	5.03	1.45	1.33
23	y	302	CHL	O2D-CGD	5.02	1.45	1.33
23	Ba	306	CHL	O2D-CGD	5.02	1.45	1.33
23	r	613	CHL	C3D-C4D	-5.02	1.32	1.44
23	BJ	609	CHL	C2C-C3C	5.02	1.47	1.36
23	A6	605	CHL	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	606	CHL	O2D-CGD	5.02	1.45	1.33
23	r	605	CHL	O2D-CGD	5.02	1.45	1.33
23	5	606	CHL	O2D-CGD	5.02	1.45	1.33
23	g	608	CHL	O2D-CGD	5.02	1.45	1.33
23	S	605	CHL	O2D-CGD	5.02	1.45	1.33
23	g	609	CHL	C2C-C3C	5.01	1.47	1.36
23	AB	306	CHL	O2D-CGD	5.01	1.45	1.33
23	7	309	CHL	O2D-CGD	5.00	1.45	1.33
23	BJ	609	CHL	CHD-C1D	5.00	1.48	1.38
23	AA	309	CHL	O2D-CGD	5.00	1.45	1.33
23	AA	306	CHL	C2C-C3C	5.00	1.47	1.36
23	A6	607	CHL	O2D-CGD	5.00	1.45	1.33
23	6	609	CHL	CHC-C1C	5.00	1.48	1.38
23	8	307	CHL	O2D-CGD	4.99	1.45	1.33
23	Ba	302	CHL	O2D-CGD	4.99	1.45	1.33
23	BU	605	CHL	O2D-CGD	4.99	1.45	1.33
23	7	306	CHL	C2C-C3C	4.98	1.47	1.36
23	BB	309	CHL	C3D-C4D	-4.98	1.32	1.44
23	Au	601	CHL	C3D-C4D	-4.98	1.32	1.44
23	0	606	CHL	O2D-CGD	4.98	1.45	1.33
23	G	609	CHL	C3D-C4D	-4.98	1.32	1.44
23	S	607	CHL	CHC-C1C	4.98	1.48	1.38
23	0	601	CHL	C3D-C4D	-4.97	1.32	1.44
23	6	601	CHL	C3D-C4D	-4.97	1.32	1.44
23	Y	302	CHL	O2D-CGD	4.97	1.45	1.33
23	s	606	CHL	O2D-CGD	4.97	1.45	1.33
23	8	307	CHL	C3D-C4D	-4.97	1.33	1.44
23	Ba	310	CHL	C2C-C3C	4.97	1.47	1.36
23	n	609	CHL	O2D-CGD	4.97	1.45	1.33
23	A2	606	CHL	O2D-CGD	4.96	1.45	1.33
23	5	608	CHL	C3D-C4D	-4.96	1.33	1.44
23	BV	606	CHL	O2D-CGD	4.96	1.45	1.33
23	N	608	CHL	C3D-C4D	-4.96	1.33	1.44
23	AB	306	CHL	C3D-C4D	-4.96	1.33	1.44
23	Y	302	CHL	C3D-C4D	-4.95	1.33	1.44
23	y	310	CHL	C2C-C3C	4.95	1.47	1.36
23	A2	608	CHL	C3D-C4D	-4.95	1.33	1.44
23	G	601	CHL	O2D-CGD	4.94	1.45	1.33
23	G	601	CHL	C3D-C4D	-4.94	1.33	1.44
23	BU	607	CHL	C3D-C4D	-4.93	1.33	1.44
23	BB	302	CHL	O2D-CGD	4.93	1.45	1.33
23	y	310	CHL	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	306	CHL	C3D-C4D	-4.92	1.33	1.44
23	Au	609	CHL	C3D-C4D	-4.92	1.33	1.44
23	8	304	CHL	O2D-CGD	4.92	1.45	1.33
23	BB	307	CHL	O2D-CGD	4.92	1.45	1.33
23	A6	607	CHL	CHC-C1C	4.91	1.48	1.38
23	N	605	CHL	O2D-CGD	4.91	1.45	1.33
23	AB	307	CHL	O2D-CGD	4.90	1.45	1.33
23	9	606	CHL	C3D-C4D	-4.90	1.33	1.44
23	r	607	CHL	C3D-C4D	-4.90	1.33	1.44
23	BU	606	CHL	C3D-C4D	-4.90	1.33	1.44
23	y	310	CHL	C3D-C4D	-4.89	1.33	1.44
23	Y	308	CHL	C3D-C4D	-4.89	1.33	1.44
23	BJ	609	CHL	CHC-C1C	4.89	1.48	1.38
23	G	609	CHL	CHD-C1D	4.89	1.47	1.38
23	6	609	CHL	O2D-CGD	4.89	1.45	1.33
23	5	606	CHL	C3D-C4D	-4.89	1.33	1.44
23	Au	608	CHL	C3D-C4D	-4.89	1.33	1.44
23	9	601	CHL	O2D-CGD	4.89	1.45	1.33
23	7	310	CHL	C3D-C4D	-4.89	1.33	1.44
23	G	608	CHL	C3D-C4D	-4.89	1.33	1.44
23	5	601	CHL	O2D-CGD	4.89	1.45	1.33
23	A2	605	CHL	C3D-C4D	-4.88	1.33	1.44
23	AB	304	CHL	O2D-CGD	4.88	1.45	1.33
23	Au	601	CHL	O2D-CGD	4.88	1.45	1.33
23	BB	308	CHL	C3D-C4D	-4.88	1.33	1.44
23	N	605	CHL	C3D-C4D	-4.88	1.33	1.44
23	N	608	CHL	O2D-CGD	4.88	1.45	1.33
23	A2	608	CHL	O2D-CGD	4.88	1.45	1.33
23	Y	307	CHL	O2D-CGD	4.87	1.45	1.33
23	Y	309	CHL	C3D-C4D	-4.87	1.33	1.44
23	5	609	CHL	O2D-CGD	4.87	1.45	1.33
23	5	607	CHL	C3D-C4D	-4.87	1.33	1.44
23	g	609	CHL	CHC-C1C	4.86	1.48	1.38
23	0	609	CHL	O2D-CGD	4.85	1.45	1.33
31	D	403	PL9	C6-C1	-4.85	1.39	1.48
23	r	606	CHL	C3D-C4D	-4.85	1.33	1.44
23	A2	606	CHL	C3D-C4D	-4.84	1.33	1.44
23	A6	606	CHL	O2D-CGD	4.84	1.45	1.33
23	A2	607	CHL	C3D-C4D	-4.84	1.33	1.44
23	A2	605	CHL	O2D-CGD	4.84	1.45	1.33
23	6	608	CHL	C3D-C4D	-4.84	1.33	1.44
23	S	606	CHL	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	310	CHL	C3D-C4D	-4.84	1.33	1.44
23	BB	306	CHL	C3D-C4D	-4.84	1.33	1.44
23	N	607	CHL	C3D-C4D	-4.83	1.33	1.44
23	5	608	CHL	O2D-CGD	4.83	1.45	1.33
23	9	607	CHL	C3D-C4D	-4.83	1.33	1.44
23	A2	601	CHL	C3D-C4D	-4.83	1.33	1.44
23	BV	605	CHL	C3D-C4D	-4.82	1.33	1.44
23	0	608	CHL	C3D-C4D	-4.82	1.33	1.44
23	Ba	310	CHL	CHD-C1D	4.82	1.47	1.38
23	AA	302	CHL	C2C-C3C	4.82	1.47	1.36
23	0	607	CHL	C3D-C4D	-4.82	1.33	1.44
23	BU	605	CHL	C3D-C4D	-4.82	1.33	1.44
23	A6	601	CHL	C3D-C4D	-4.81	1.33	1.44
23	y	310	CHL	CHD-C1D	4.81	1.47	1.38
23	8	305	CHL	C3D-C4D	-4.81	1.33	1.44
23	N	606	CHL	C3D-C4D	-4.81	1.33	1.44
23	Y	307	CHL	C3D-C4D	-4.81	1.33	1.44
23	N	601	CHL	C3D-C4D	-4.81	1.33	1.44
23	s	605	CHL	C3D-C4D	-4.81	1.33	1.44
23	BB	307	CHL	C3D-C4D	-4.81	1.33	1.44
23	s	607	CHL	C2C-C3C	4.81	1.47	1.36
23	Ba	310	CHL	CHC-C1C	4.81	1.48	1.38
31	d	403	PL9	C26-C24	-4.81	1.41	1.51
23	BV	607	CHL	C2C-C3C	4.80	1.47	1.36
23	g	609	CHL	C3D-C4D	-4.80	1.33	1.44
23	9	609	CHL	O2D-CGD	4.80	1.44	1.33
23	y	310	CHL	CHC-C1C	4.80	1.48	1.38
23	BJ	609	CHL	C3D-C4D	-4.80	1.33	1.44
23	6	601	CHL	O2D-CGD	4.80	1.44	1.33
28	AA	301	XAT	C8-C9	4.80	1.56	1.45
28	7	301	XAT	C8-C9	4.80	1.56	1.45
23	6	607	CHL	C3D-C4D	-4.80	1.33	1.44
23	r	605	CHL	C3D-C4D	-4.79	1.33	1.44
23	AB	305	CHL	C3D-C4D	-4.79	1.33	1.44
23	Ba	302	CHL	C3D-C4D	-4.79	1.33	1.44
23	7	302	CHL	C2C-C3C	4.79	1.47	1.36
23	Y	306	CHL	C3D-C4D	-4.79	1.33	1.44
23	AA	306	CHL	CHC-C1C	4.78	1.48	1.38
23	0	601	CHL	O2D-CGD	4.78	1.44	1.33
23	S	601	CHL	C3D-C4D	-4.78	1.33	1.44
23	y	302	CHL	C3D-C4D	-4.78	1.33	1.44
23	8	304	CHL	C3D-C4D	-4.77	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	306	CHL	CHD-C1D	4.77	1.47	1.38
23	A6	607	CHL	C3D-C4D	-4.77	1.33	1.44
23	5	601	CHL	C3D-C4D	-4.77	1.33	1.44
23	Ba	310	CHL	C3D-C4D	-4.77	1.33	1.44
28	Au	619	XAT	C8-C9	4.76	1.56	1.45
23	Y	309	CHL	O2D-CGD	4.76	1.44	1.33
23	n	609	CHL	C3D-C4D	-4.75	1.33	1.44
28	BB	301	XAT	C28-C29	4.75	1.56	1.45
28	8	312	XAT	C8-C9	4.75	1.56	1.45
23	S	606	CHL	C3D-C4D	-4.75	1.33	1.44
23	7	306	CHL	CHD-C1D	4.75	1.47	1.38
23	A6	606	CHL	C3D-C4D	-4.75	1.33	1.44
26	A2	617	NEX	C10-C9	4.75	1.42	1.35
23	AB	304	CHL	C3D-C4D	-4.75	1.33	1.44
23	9	601	CHL	C3D-C4D	-4.74	1.33	1.44
23	0	606	CHL	C3D-C4D	-4.74	1.33	1.44
28	AB	312	XAT	C8-C9	4.74	1.56	1.45
23	BQ	609	CHL	C3D-C4D	-4.74	1.33	1.44
23	AA	309	CHL	C3D-C4D	-4.74	1.33	1.44
23	AA	310	CHL	CHD-C1D	4.74	1.47	1.38
23	7	307	CHL	C3D-C4D	-4.73	1.33	1.44
23	BV	601	CHL	C3D-C4D	-4.73	1.33	1.44
23	AB	307	CHL	CHD-C1D	4.73	1.47	1.38
23	9	605	CHL	C3D-C4D	-4.73	1.33	1.44
23	N	609	CHL	O2D-CGD	4.73	1.44	1.33
23	AA	302	CHL	C3D-C4D	-4.73	1.33	1.44
23	G	607	CHL	C3D-C4D	-4.73	1.33	1.44
23	7	302	CHL	C3D-C4D	-4.73	1.33	1.44
23	7	306	CHL	CHC-C1C	4.72	1.48	1.38
23	Ba	306	CHL	C3D-C4D	-4.72	1.33	1.44
23	AA	307	CHL	C3D-C4D	-4.72	1.33	1.44
23	BJ	605	CHL	C2C-C3C	4.72	1.46	1.36
23	r	613	CHL	O2D-CGD	4.72	1.44	1.33
23	6	606	CHL	C3D-C4D	-4.71	1.33	1.44
23	7	309	CHL	C3D-C4D	-4.71	1.33	1.44
23	0	605	CHL	C3D-C4D	-4.71	1.33	1.44
23	s	601	CHL	C3D-C4D	-4.71	1.33	1.44
23	7	310	CHL	CHD-C1D	4.71	1.47	1.38
23	5	607	CHL	O2D-CGD	4.71	1.44	1.33
31	BG	403	PL9	C3-C4	-4.71	1.41	1.49
23	n	601	CHL	C2C-C3C	4.71	1.46	1.36
23	A2	609	CHL	O2D-CGD	4.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	605	CHL	C3D-C4D	-4.70	1.33	1.44
23	AA	308	CHL	C3D-C4D	-4.70	1.33	1.44
28	G	619	XAT	C8-C9	4.70	1.56	1.45
28	g	619	XAT	C8-C9	4.70	1.56	1.45
23	9	608	CHL	O2D-CGD	4.70	1.44	1.33
23	BJ	607	CHL	C2C-C3C	4.70	1.46	1.36
23	Au	605	CHL	C2C-C3C	4.70	1.46	1.36
23	BU	613	CHL	O2D-CGD	4.70	1.44	1.33
23	9	609	CHL	CHD-C1D	4.70	1.47	1.38
23	y	306	CHL	C3D-C4D	-4.70	1.33	1.44
28	Y	301	XAT	C8-C9	4.70	1.56	1.45
23	AA	307	CHL	C2C-C3C	4.70	1.46	1.36
23	S	607	CHL	C3D-C4D	-4.70	1.33	1.44
32	BO	101	SQD	O48-C23	4.69	1.47	1.33
28	BB	301	XAT	C8-C9	4.69	1.56	1.45
32	a	412	SQD	O48-C23	4.69	1.47	1.33
23	G	605	CHL	C2C-C3C	4.69	1.46	1.36
23	A6	605	CHL	C3D-C4D	-4.69	1.33	1.44
23	6	605	CHL	C3D-C4D	-4.69	1.33	1.44
32	BG	406	SQD	O48-C23	4.69	1.47	1.33
23	Au	607	CHL	C3D-C4D	-4.68	1.33	1.44
23	7	308	CHL	C3D-C4D	-4.68	1.33	1.44
23	7	307	CHL	C2C-C3C	4.68	1.46	1.36
28	7	318	XAT	C8-C9	4.68	1.56	1.45
28	BJ	619	XAT	C8-C9	4.68	1.56	1.45
23	e	601	CHL	C3D-C4D	-4.68	1.33	1.44
23	g	605	CHL	C2C-C3C	4.68	1.46	1.36
28	Y	301	XAT	C28-C29	4.68	1.56	1.45
23	Au	606	CHL	C3D-C4D	-4.68	1.33	1.44
32	l	101	SQD	O48-C23	4.68	1.47	1.33
28	AA	318	XAT	C8-C9	4.68	1.56	1.45
23	S	605	CHL	C3D-C4D	-4.67	1.33	1.44
23	g	606	CHL	C2C-C3C	4.67	1.46	1.36
23	BQ	606	CHL	CHC-C1C	4.67	1.48	1.38
32	BD	412	SQD	O48-C23	4.67	1.47	1.33
23	BB	308	CHL	O2A-CGA	4.67	1.47	1.33
23	g	607	CHL	C2C-C3C	4.67	1.46	1.36
28	n	619	XAT	C8-C9	4.66	1.56	1.45
23	BH	601	CHL	C3D-C4D	-4.66	1.33	1.44
23	s	601	CHL	CHC-C1C	4.65	1.48	1.38
23	BV	601	CHL	CHC-C1C	4.65	1.48	1.38
23	BQ	601	CHL	C2C-C3C	4.65	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	302	CHL	CHC-C1C	4.65	1.48	1.38
23	N	606	CHL	CHC-C1C	4.65	1.48	1.38
23	Y	308	CHL	O2A-CGA	4.65	1.46	1.33
23	7	302	CHL	CHC-C1C	4.65	1.48	1.38
32	d	406	SQD	O48-C23	4.65	1.46	1.33
23	BQ	608	CHL	C3D-C4D	-4.65	1.33	1.44
23	9	605	CHL	C2C-C3C	4.64	1.46	1.36
23	5	605	CHL	C2C-C3C	4.64	1.46	1.36
23	BH	601	CHL	O2D-CGD	4.64	1.45	1.30
23	G	608	CHL	O2D-CGD	4.64	1.44	1.33
23	y	309	CHL	C2C-C3C	4.64	1.46	1.36
23	0	608	CHL	O2D-CGD	4.64	1.44	1.33
23	e	601	CHL	O2D-CGD	4.64	1.45	1.30
28	Au	619	XAT	C28-C29	4.64	1.55	1.45
23	BU	606	CHL	O2A-CGA	4.64	1.46	1.33
23	Au	608	CHL	O2D-CGD	4.63	1.44	1.33
23	6	608	CHL	O2D-CGD	4.63	1.44	1.33
28	A2	619	XAT	C8-C9	4.63	1.55	1.45
23	Y	310	CHL	O2D-CGD	4.63	1.44	1.33
23	n	608	CHL	C3D-C4D	-4.63	1.33	1.44
23	y	308	CHL	C3D-C4D	-4.63	1.33	1.44
23	n	607	CHL	C3D-C4D	-4.63	1.33	1.44
23	y	309	CHL	CHC-C1C	4.63	1.47	1.38
23	Ba	309	CHL	CHC-C1C	4.62	1.47	1.38
23	A2	606	CHL	CHC-C1C	4.62	1.47	1.38
23	Ba	308	CHL	C3D-C4D	-4.62	1.33	1.44
23	G	606	CHL	C3D-C4D	-4.62	1.33	1.44
23	BJ	606	CHL	C2C-C3C	4.62	1.46	1.36
23	BV	607	CHL	CHC-C1C	4.62	1.47	1.38
28	G	619	XAT	C28-C29	4.61	1.55	1.45
32	D	406	SQD	O48-C23	4.61	1.46	1.33
25	BJ	616	LUT	C14-C13	4.61	1.41	1.35
23	BB	309	CHL	O2D-CGD	4.61	1.44	1.33
23	BQ	607	CHL	C3D-C4D	-4.60	1.33	1.44
23	AA	302	CHL	CHD-C1D	4.60	1.47	1.38
23	g	601	CHL	C3D-C4D	-4.60	1.33	1.44
23	n	608	CHL	C2C-C3C	4.60	1.46	1.36
28	A2	619	XAT	C28-C29	4.60	1.55	1.45
23	y	306	CHL	C2C-C3C	4.60	1.46	1.36
23	5	601	CHL	C2C-C3C	4.60	1.46	1.36
23	g	607	CHL	C3D-C4D	-4.60	1.33	1.44
28	BQ	619	XAT	C8-C9	4.60	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	r	616	XAT	C28-C29	4.59	1.55	1.45
28	N	619	XAT	C28-C29	4.59	1.55	1.45
28	BJ	619	XAT	C28-C29	4.59	1.55	1.45
23	r	606	CHL	O2A-CGA	4.59	1.46	1.33
28	N	619	XAT	C8-C9	4.59	1.55	1.45
23	8	306	CHL	C2C-C3C	4.59	1.46	1.36
23	BQ	601	CHL	C3D-C4D	-4.59	1.33	1.44
23	s	607	CHL	CHC-C1C	4.59	1.47	1.38
28	g	619	XAT	C28-C29	4.59	1.55	1.45
23	g	605	CHL	C3D-C4D	-4.59	1.33	1.44
23	8	304	CHL	C2C-C3C	4.58	1.46	1.36
32	l	102	SQD	O48-C23	4.58	1.46	1.33
32	BO	102	SQD	O48-C23	4.58	1.46	1.33
23	r	607	CHL	O2D-CGD	4.58	1.44	1.33
23	n	606	CHL	CHC-C1C	4.58	1.47	1.38
23	BJ	608	CHL	C3D-C4D	-4.58	1.33	1.44
28	7	301	XAT	C32-C33	4.58	1.55	1.45
23	8	306	CHL	CHC-C1C	4.58	1.47	1.38
23	n	601	CHL	C3D-C4D	-4.58	1.33	1.44
23	BQ	608	CHL	C2C-C3C	4.58	1.46	1.36
28	BU	616	XAT	C28-C29	4.57	1.55	1.45
23	AB	306	CHL	CHC-C1C	4.57	1.47	1.38
23	Ba	309	CHL	C2C-C3C	4.57	1.46	1.36
23	9	601	CHL	C2C-C3C	4.57	1.46	1.36
32	L	103	SQD	O48-C23	4.57	1.46	1.33
23	9	607	CHL	O2D-CGD	4.57	1.44	1.33
28	7	301	XAT	C28-C29	4.57	1.55	1.45
23	Ba	307	CHL	C3D-C4D	-4.56	1.33	1.44
23	g	608	CHL	C3D-C4D	-4.56	1.33	1.44
29	BF	516	BCR	C30-C25	-4.56	1.47	1.53
23	BJ	605	CHL	C3D-C4D	-4.56	1.33	1.44
23	BJ	601	CHL	C3D-C4D	-4.56	1.33	1.44
25	5	616	LUT	C34-C33	4.55	1.41	1.35
23	n	608	CHL	CHC-C1C	4.55	1.47	1.38
23	y	307	CHL	C3D-C4D	-4.55	1.33	1.44
28	n	619	XAT	C28-C29	4.55	1.55	1.45
23	0	609	CHL	CHD-C1D	4.55	1.47	1.38
23	AA	310	CHL	C2C-C3C	4.55	1.46	1.36
23	Ba	307	CHL	CHC-C1C	4.55	1.47	1.38
23	AB	306	CHL	C2C-C3C	4.55	1.46	1.36
23	BQ	606	CHL	C3D-C4D	-4.55	1.33	1.44
23	A2	607	CHL	O2A-CGA	4.55	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	609	CHL	CHD-C1D	4.55	1.47	1.38
28	AA	301	XAT	C32-C33	4.55	1.55	1.45
28	y	301	XAT	C28-C29	4.55	1.55	1.45
23	Ba	309	CHL	C3D-C4D	-4.55	1.33	1.44
23	n	605	CHL	C2C-C3C	4.55	1.46	1.36
32	A	413	SQD	O48-C23	4.55	1.46	1.33
23	y	307	CHL	CHC-C1C	4.55	1.47	1.38
23	AB	304	CHL	C2C-C3C	4.55	1.46	1.36
28	BQ	619	XAT	C28-C29	4.55	1.55	1.45
32	Az	101	SQD	O48-C23	4.54	1.46	1.33
23	6	609	CHL	C2C-C3C	4.54	1.46	1.36
23	5	601	CHL	O2A-CGA	4.54	1.46	1.30
23	Au	605	CHL	O2A-CGA	4.54	1.46	1.30
32	R	411	SQD	O48-C23	4.54	1.46	1.33
23	AB	304	CHL	O2A-CGA	4.54	1.46	1.30
23	7	306	CHL	C3D-C4D	-4.54	1.33	1.44
28	Ba	301	XAT	C8-C9	4.54	1.55	1.45
23	7	309	CHL	C2C-C3C	4.54	1.46	1.36
23	BQ	608	CHL	CHC-C1C	4.54	1.47	1.38
23	8	304	CHL	O2A-CGA	4.54	1.46	1.30
23	BV	605	CHL	CHC-C1C	4.54	1.47	1.38
23	Ba	306	CHL	C2C-C3C	4.53	1.46	1.36
23	BJ	607	CHL	C3D-C4D	-4.53	1.33	1.44
32	A1	101	SQD	O48-C23	4.53	1.46	1.33
23	7	302	CHL	CHD-C1D	4.53	1.47	1.38
23	8	307	CHL	CHD-C1D	4.53	1.47	1.38
25	7	316	LUT	C14-C13	4.53	1.41	1.35
23	G	609	CHL	CHC-C1C	4.53	1.47	1.38
23	G	605	CHL	O2A-CGA	4.53	1.46	1.30
23	n	606	CHL	C3D-C4D	-4.53	1.34	1.44
23	s	607	CHL	O2A-CGA	4.53	1.46	1.30
23	BU	607	CHL	O2D-CGD	4.53	1.44	1.33
23	n	608	CHL	CHD-C1D	4.53	1.47	1.38
23	7	310	CHL	C2C-C3C	4.53	1.46	1.36
28	AA	301	XAT	C28-C29	4.53	1.55	1.45
28	y	301	XAT	C8-C9	4.53	1.55	1.45
23	6	605	CHL	C2C-C3C	4.53	1.46	1.36
23	BQ	607	CHL	C2C-C3C	4.53	1.46	1.36
23	BQ	605	CHL	C3D-C4D	-4.53	1.34	1.44
23	BV	601	CHL	O2A-CGA	4.53	1.46	1.30
23	Ba	309	CHL	CHD-C1D	4.52	1.47	1.38
28	AA	301	XAT	C12-C13	4.52	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	307	CHL	O2A-CGA	4.52	1.45	1.30
23	0	606	CHL	O2A-CGA	4.52	1.45	1.30
23	AA	309	CHL	O2A-CGA	4.52	1.45	1.30
23	7	307	CHL	O2A-CGA	4.52	1.45	1.30
23	6	606	CHL	O2A-CGA	4.52	1.45	1.30
23	AA	309	CHL	C2C-C3C	4.52	1.46	1.36
23	e	601	CHL	C2C-C3C	4.52	1.46	1.36
23	0	607	CHL	C2C-C3C	4.52	1.46	1.36
23	BH	601	CHL	C2C-C3C	4.52	1.46	1.36
23	Ba	308	CHL	C2C-C3C	4.52	1.46	1.36
23	n	605	CHL	C3D-C4D	-4.52	1.34	1.44
28	Ba	301	XAT	C28-C29	4.52	1.55	1.45
23	9	601	CHL	O2A-CGA	4.52	1.45	1.30
23	S	601	CHL	O2A-CGA	4.51	1.45	1.30
23	BJ	601	CHL	C2C-C3C	4.51	1.46	1.36
23	BU	613	CHL	C3A-C2A	-4.51	1.50	1.54
23	7	309	CHL	O2A-CGA	4.51	1.45	1.30
23	s	601	CHL	O2A-CGA	4.51	1.45	1.30
23	Au	605	CHL	C3D-C4D	-4.51	1.34	1.44
23	A6	601	CHL	O2A-CGA	4.51	1.45	1.30
23	BV	607	CHL	C3D-C4D	-4.51	1.34	1.44
23	AA	306	CHL	O2A-CGA	4.51	1.45	1.30
23	7	306	CHL	O2A-CGA	4.51	1.45	1.30
23	n	607	CHL	C2C-C3C	4.51	1.46	1.36
23	5	609	CHL	CHD-C1D	4.51	1.47	1.38
23	y	302	CHL	C2C-C3C	4.51	1.46	1.36
23	0	605	CHL	O2A-CGA	4.50	1.45	1.30
23	s	606	CHL	C3D-C4D	-4.50	1.34	1.44
23	AA	306	CHL	C3D-C4D	-4.50	1.34	1.44
23	0	605	CHL	CHC-C1C	4.50	1.47	1.38
28	7	301	XAT	C12-C13	4.50	1.55	1.45
23	y	309	CHL	CHD-C1D	4.50	1.47	1.38
23	G	606	CHL	C2C-C3C	4.50	1.46	1.36
23	BV	607	CHL	O2A-CGA	4.50	1.45	1.30
23	s	607	CHL	CHD-C1D	4.50	1.47	1.38
23	BV	605	CHL	C2C-C3C	4.50	1.46	1.36
23	g	606	CHL	CHD-C1D	4.50	1.47	1.38
23	7	302	CHL	O2A-CGA	4.50	1.45	1.30
23	BV	606	CHL	C3D-C4D	-4.50	1.34	1.44
23	g	606	CHL	C3D-C4D	-4.50	1.34	1.44
32	L	101	SQD	O48-C23	4.50	1.46	1.33
23	8	307	CHL	O2A-CGA	4.50	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BJ	606	CHL	C3D-C4D	-4.50	1.34	1.44
23	BQ	609	CHL	C2C-C3C	4.49	1.46	1.36
23	BJ	606	CHL	CHC-C1C	4.49	1.47	1.38
23	6	605	CHL	O2A-CGA	4.49	1.45	1.30
23	s	605	CHL	C2C-C3C	4.49	1.46	1.36
23	BQ	608	CHL	CHD-C1D	4.49	1.47	1.38
23	e	601	CHL	O2A-CGA	4.49	1.45	1.30
23	Au	606	CHL	O2A-CGA	4.49	1.46	1.33
23	BQ	601	CHL	CHD-C1D	4.49	1.47	1.38
23	BH	601	CHL	O2A-CGA	4.49	1.45	1.30
25	5	615	LUT	C34-C33	4.49	1.41	1.35
23	0	605	CHL	C2C-C3C	4.49	1.46	1.36
28	r	616	XAT	C8-C9	4.49	1.55	1.45
23	AB	307	CHL	O2A-CGA	4.48	1.45	1.30
23	AB	307	CHL	C2C-C3C	4.48	1.46	1.36
23	S	605	CHL	O2A-CGA	4.48	1.45	1.30
23	9	608	CHL	O2A-CGA	4.48	1.45	1.30
23	BQ	605	CHL	C2C-C3C	4.48	1.46	1.36
23	G	605	CHL	C3D-C4D	-4.48	1.34	1.44
23	A6	605	CHL	O2A-CGA	4.48	1.45	1.30
23	s	606	CHL	C2C-C3C	4.48	1.46	1.36
23	g	606	CHL	CHC-C1C	4.48	1.47	1.38
23	n	601	CHL	CHC-C1C	4.47	1.47	1.38
23	5	606	CHL	O2A-CGA	4.47	1.45	1.30
23	5	605	CHL	O2A-CGA	4.47	1.45	1.30
23	Au	606	CHL	C2C-C3C	4.47	1.46	1.36
23	6	605	CHL	CHC-C1C	4.47	1.47	1.38
23	G	605	CHL	CHC-C1C	4.47	1.47	1.38
23	AA	302	CHL	O2A-CGA	4.47	1.45	1.30
23	g	606	CHL	O2A-CGA	4.47	1.46	1.33
23	BV	607	CHL	CHD-C1D	4.47	1.47	1.38
23	9	606	CHL	O2A-CGA	4.47	1.45	1.30
23	g	601	CHL	C2C-C3C	4.47	1.46	1.36
23	AB	305	CHL	O2A-CGA	4.47	1.45	1.30
23	s	607	CHL	C3D-C4D	-4.47	1.34	1.44
28	AA	318	XAT	C28-C29	4.47	1.55	1.45
23	s	605	CHL	CHC-C1C	4.47	1.47	1.38
23	Ba	307	CHL	CHD-C1D	4.47	1.47	1.38
23	A6	607	CHL	C2C-C3C	4.47	1.46	1.36
23	y	307	CHL	CHD-C1D	4.46	1.47	1.38
23	BJ	606	CHL	O2A-CGA	4.46	1.46	1.33
23	5	608	CHL	O2A-CGA	4.46	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	601	CHL	C2C-C3C	4.46	1.46	1.36
28	9	619	XAT	C8-C9	4.46	1.55	1.45
28	8	312	XAT	C32-C33	4.46	1.55	1.45
23	6	608	CHL	CHC-C1C	4.46	1.47	1.38
23	N	607	CHL	O2A-CGA	4.46	1.46	1.33
23	8	305	CHL	O2A-CGA	4.46	1.45	1.30
23	BV	605	CHL	O2A-CGA	4.46	1.45	1.30
23	s	605	CHL	O2A-CGA	4.46	1.45	1.30
23	s	601	CHL	CHD-C1D	4.46	1.47	1.38
23	9	605	CHL	O2A-CGA	4.46	1.45	1.30
23	BJ	605	CHL	O2A-CGA	4.46	1.45	1.30
28	BU	616	XAT	C8-C9	4.45	1.55	1.45
23	G	606	CHL	O2A-CGA	4.45	1.46	1.33
23	AA	310	CHL	CHC-C1C	4.45	1.47	1.38
23	n	601	CHL	CHD-C1D	4.45	1.47	1.38
28	7	318	XAT	C28-C29	4.45	1.55	1.45
32	2	408	SQD	O48-C23	4.45	1.46	1.33
23	y	308	CHL	C2C-C3C	4.45	1.46	1.36
23	BB	310	CHL	O2D-CGD	4.45	1.44	1.33
23	BJ	606	CHL	CHD-C1D	4.45	1.47	1.38
23	n	609	CHL	CHD-C1D	4.45	1.47	1.38
23	BQ	601	CHL	CHC-C1C	4.44	1.47	1.38
28	AB	312	XAT	C32-C33	4.44	1.55	1.45
23	7	308	CHL	C2C-C3C	4.44	1.46	1.36
28	AB	312	XAT	C28-C29	4.44	1.55	1.45
23	g	605	CHL	O2A-CGA	4.44	1.45	1.30
23	r	613	CHL	C3A-C2A	-4.44	1.50	1.54
23	n	609	CHL	CHC-C1C	4.44	1.47	1.38
23	8	304	CHL	CHD-C1D	4.44	1.47	1.38
23	AA	308	CHL	C2C-C3C	4.44	1.46	1.36
23	A2	601	CHL	O2A-CGA	4.44	1.46	1.33
23	0	608	CHL	CHC-C1C	4.44	1.47	1.38
23	S	607	CHL	O2A-CGA	4.44	1.45	1.30
23	S	606	CHL	O2A-CGA	4.43	1.46	1.33
23	BB	310	CHL	O2A-CGA	4.43	1.46	1.33
23	AB	304	CHL	CHD-C1D	4.43	1.47	1.38
23	A2	609	CHL	O2A-CGA	4.43	1.46	1.33
23	y	309	CHL	C3D-C4D	-4.43	1.34	1.44
23	BJ	605	CHL	CHC-C1C	4.43	1.47	1.38
23	BQ	609	CHL	CHD-C1D	4.43	1.47	1.38
23	y	302	CHL	O2A-CGA	4.43	1.46	1.33
28	9	619	XAT	C28-C29	4.43	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BV	606	CHL	C2C-C3C	4.43	1.46	1.36
23	N	606	CHL	O2A-CGA	4.42	1.46	1.33
23	BJ	608	CHL	C2C-C3C	4.42	1.46	1.36
23	S	601	CHL	CHC-C1C	4.42	1.47	1.38
23	6	608	CHL	O2A-CGA	4.42	1.45	1.30
23	G	608	CHL	CHD-C1D	4.42	1.47	1.38
23	5	605	CHL	CHD-C1D	4.42	1.47	1.38
23	g	608	CHL	C2C-C3C	4.42	1.46	1.36
23	7	310	CHL	CHC-C1C	4.42	1.47	1.38
23	BV	601	CHL	C2C-C3C	4.42	1.46	1.36
26	AA	319	NEX	C14-C13	4.42	1.41	1.35
23	g	605	CHL	CHC-C1C	4.42	1.47	1.38
28	g	619	XAT	C12-C13	4.42	1.55	1.45
23	0	608	CHL	O2A-CGA	4.42	1.45	1.30
23	n	606	CHL	O2A-CGA	4.42	1.46	1.33
28	BJ	619	XAT	C12-C13	4.42	1.55	1.45
23	BQ	606	CHL	O2A-CGA	4.42	1.46	1.33
23	Ba	302	CHL	C2C-C3C	4.42	1.46	1.36
23	Y	310	CHL	O2A-CGA	4.41	1.46	1.33
23	A6	607	CHL	CHD-C1D	4.41	1.47	1.38
23	A2	606	CHL	O2A-CGA	4.41	1.46	1.33
23	n	607	CHL	CHC-C1C	4.41	1.47	1.38
23	S	606	CHL	C2C-C3C	4.41	1.46	1.36
23	n	609	CHL	C2C-C3C	4.41	1.46	1.36
28	5	619	XAT	C28-C29	4.41	1.55	1.45
23	r	606	CHL	C2C-C3C	4.41	1.46	1.36
23	BQ	606	CHL	C2C-C3C	4.41	1.46	1.36
23	9	605	CHL	CHD-C1D	4.41	1.46	1.38
23	N	601	CHL	O2A-CGA	4.41	1.46	1.33
28	8	312	XAT	C28-C29	4.40	1.55	1.45
23	n	601	CHL	O2A-CGA	4.40	1.46	1.33
23	A6	606	CHL	O2A-CGA	4.40	1.46	1.33
28	n	619	XAT	C12-C13	4.40	1.55	1.45
23	BU	607	CHL	C2C-C3C	4.40	1.46	1.36
28	7	318	XAT	C12-C13	4.40	1.55	1.45
23	6	607	CHL	C2C-C3C	4.40	1.46	1.36
23	A6	601	CHL	CHC-C1C	4.40	1.47	1.38
23	G	606	CHL	CHC-C1C	4.40	1.47	1.38
23	BQ	606	CHL	CHD-C1D	4.40	1.46	1.38
23	9	601	CHL	CHC-C1C	4.40	1.47	1.38
26	7	319	NEX	C14-C13	4.40	1.41	1.35
23	g	607	CHL	CHD-C1D	4.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Ba	306	CHL	CHD-C1D	4.40	1.46	1.38
28	Au	619	XAT	C32-C33	4.39	1.55	1.45
28	BB	301	XAT	C32-C33	4.39	1.55	1.45
23	y	302	CHL	CHD-C1D	4.39	1.46	1.38
23	y	306	CHL	CHC-C1C	4.39	1.47	1.38
23	9	606	CHL	C2C-C3C	4.39	1.46	1.36
23	Ba	302	CHL	O2A-CGA	4.39	1.46	1.33
26	BJ	617	NEX	C14-C13	4.39	1.41	1.35
23	Y	306	CHL	CHC-C1C	4.39	1.47	1.38
23	Au	608	CHL	CHD-C1D	4.39	1.46	1.38
23	BQ	609	CHL	CHC-C1C	4.39	1.47	1.38
23	s	605	CHL	CHD-C1D	4.39	1.46	1.38
23	BV	601	CHL	CHD-C1D	4.39	1.46	1.38
23	y	307	CHL	O2A-CGA	4.39	1.46	1.33
23	A6	607	CHL	O2A-CGA	4.39	1.45	1.30
23	y	307	CHL	C2C-C3C	4.39	1.46	1.36
28	G	619	XAT	C32-C33	4.39	1.55	1.45
23	BQ	601	CHL	O2A-CGA	4.39	1.46	1.33
23	BB	306	CHL	CHC-C1C	4.39	1.47	1.38
23	8	305	CHL	C2C-C3C	4.39	1.46	1.36
23	y	306	CHL	CHD-C1D	4.39	1.46	1.38
23	N	609	CHL	O2A-CGA	4.39	1.46	1.33
28	5	619	XAT	C8-C9	4.38	1.55	1.45
23	Ba	302	CHL	CHD-C1D	4.38	1.46	1.38
28	AA	318	XAT	C32-C33	4.38	1.55	1.45
23	6	601	CHL	CHD-C1D	4.38	1.46	1.38
23	BQ	607	CHL	CHC-C1C	4.38	1.47	1.38
23	s	606	CHL	O2A-CGA	4.38	1.46	1.33
25	5	615	LUT	C14-C13	4.38	1.41	1.35
23	Au	606	CHL	CHC-C1C	4.38	1.47	1.38
23	Y	310	CHL	CHD-C1D	4.38	1.46	1.38
23	5	601	CHL	CHC-C1C	4.38	1.47	1.38
23	Au	605	CHL	CHD-C1D	4.38	1.46	1.38
23	Y	307	CHL	O2A-CGA	4.37	1.46	1.33
23	8	307	CHL	C2C-C3C	4.37	1.46	1.36
23	6	605	CHL	CHD-C1D	4.37	1.46	1.38
23	BV	605	CHL	CHD-C1D	4.37	1.46	1.38
23	BB	307	CHL	O2A-CGA	4.37	1.46	1.33
23	Ba	306	CHL	CHC-C1C	4.37	1.47	1.38
23	BJ	608	CHL	CHD-C1D	4.37	1.46	1.38
23	Ba	307	CHL	O2A-CGA	4.37	1.46	1.33
23	Ba	308	CHL	CHC-C1C	4.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	307	CHL	CHC-C1C	4.37	1.47	1.38
23	5	605	CHL	CHC-C1C	4.37	1.47	1.38
23	A6	606	CHL	C2C-C3C	4.37	1.46	1.36
23	0	601	CHL	CHD-C1D	4.37	1.46	1.38
23	0	607	CHL	CHD-C1D	4.37	1.46	1.38
23	g	608	CHL	CHD-C1D	4.36	1.46	1.38
23	5	606	CHL	C2C-C3C	4.36	1.46	1.36
23	Ba	307	CHL	C2C-C3C	4.36	1.46	1.36
23	7	309	CHL	CHD-C1D	4.36	1.46	1.38
23	y	308	CHL	CHC-C1C	4.36	1.47	1.38
25	g	616	LUT	C14-C13	4.36	1.41	1.35
23	6	608	CHL	CHD-C1D	4.36	1.46	1.38
23	9	606	CHL	CHD-C1D	4.36	1.46	1.38
28	Y	301	XAT	C32-C33	4.36	1.55	1.45
23	AB	305	CHL	C2C-C3C	4.36	1.46	1.36
23	0	608	CHL	CHD-C1D	4.36	1.46	1.38
23	r	607	CHL	C2C-C3C	4.35	1.46	1.36
23	0	605	CHL	CHD-C1D	4.35	1.46	1.38
23	Ba	302	CHL	CHC-C1C	4.35	1.47	1.38
23	Ba	308	CHL	CHD-C1D	4.35	1.46	1.38
28	BQ	619	XAT	C12-C13	4.35	1.55	1.45
23	BV	606	CHL	O2A-CGA	4.35	1.46	1.33
23	n	607	CHL	O2A-CGA	4.35	1.46	1.33
23	n	605	CHL	CHC-C1C	4.35	1.47	1.38
23	BU	606	CHL	C2C-C3C	4.35	1.46	1.36
28	7	318	XAT	C32-C33	4.35	1.55	1.45
23	N	605	CHL	C2C-C3C	4.35	1.46	1.36
23	BQ	607	CHL	O2A-CGA	4.35	1.46	1.33
23	S	605	CHL	CHC-C1C	4.35	1.47	1.38
23	n	606	CHL	C2C-C3C	4.34	1.46	1.36
23	n	606	CHL	CHD-C1D	4.34	1.46	1.38
23	Au	605	CHL	CHC-C1C	4.34	1.47	1.38
23	BB	310	CHL	CHD-C1D	4.34	1.46	1.38
23	5	607	CHL	C2C-C3C	4.34	1.46	1.36
23	n	607	CHL	CHD-C1D	4.34	1.46	1.38
28	AA	318	XAT	C12-C13	4.34	1.55	1.45
23	y	302	CHL	CHC-C1C	4.34	1.47	1.38
23	g	601	CHL	O2A-CGA	4.34	1.46	1.33
26	G	617	NEX	C14-C13	4.34	1.41	1.35
23	BJ	607	CHL	CHD-C1D	4.34	1.46	1.38
23	BJ	607	CHL	CHC-C1C	4.34	1.47	1.38
23	BQ	607	CHL	CHD-C1D	4.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BJ	601	CHL	O2A-CGA	4.34	1.46	1.33
23	BV	606	CHL	CHC-C1C	4.34	1.47	1.38
23	BB	309	CHL	CHC-C1C	4.33	1.47	1.38
23	Y	306	CHL	C2C-C3C	4.33	1.46	1.36
23	8	306	CHL	CHD-C1D	4.33	1.46	1.38
23	AA	309	CHL	CHD-C1D	4.33	1.46	1.38
26	g	617	NEX	C14-C13	4.33	1.41	1.35
26	Au	617	NEX	C34-C33	4.33	1.41	1.35
23	BQ	605	CHL	CHC-C1C	4.33	1.47	1.38
28	n	619	XAT	C32-C33	4.33	1.55	1.45
23	g	607	CHL	CHC-C1C	4.33	1.47	1.38
28	9	619	XAT	C12-C13	4.33	1.55	1.45
23	Au	601	CHL	O2A-CGA	4.33	1.46	1.33
28	G	619	XAT	C12-C13	4.32	1.55	1.45
23	G	601	CHL	O2A-CGA	4.32	1.46	1.33
28	r	616	XAT	C32-C33	4.32	1.55	1.45
23	AA	307	CHL	CHD-C1D	4.32	1.46	1.38
23	r	605	CHL	O2A-CGA	4.32	1.46	1.33
23	9	605	CHL	CHC-C1C	4.32	1.47	1.38
23	G	607	CHL	CHC-C1C	4.32	1.47	1.38
23	BU	606	CHL	CHC-C1C	4.32	1.47	1.38
23	Ba	308	CHL	O2A-CGA	4.32	1.46	1.33
28	Au	619	XAT	C12-C13	4.32	1.55	1.45
23	Au	608	CHL	CHC-C1C	4.31	1.47	1.38
23	5	606	CHL	CHD-C1D	4.31	1.46	1.38
23	y	308	CHL	CHD-C1D	4.31	1.46	1.38
23	BB	306	CHL	C2C-C3C	4.31	1.46	1.36
23	G	608	CHL	CHC-C1C	4.31	1.47	1.38
23	G	606	CHL	CHD-C1D	4.31	1.46	1.38
23	g	607	CHL	O2A-CGA	4.31	1.45	1.33
23	n	605	CHL	O2A-CGA	4.31	1.45	1.33
23	5	609	CHL	CHC-C4B	4.31	1.49	1.39
26	AA	319	NEX	C30-C29	4.31	1.41	1.35
28	Ba	301	XAT	C12-C13	4.30	1.55	1.45
23	6	601	CHL	C2C-C3C	4.30	1.46	1.36
23	6	601	CHL	O2A-CGA	4.30	1.45	1.33
28	BJ	619	XAT	C32-C33	4.30	1.55	1.45
23	Y	309	CHL	CHC-C1C	4.30	1.47	1.38
23	g	601	CHL	CHD-C1D	4.30	1.46	1.38
23	BU	613	CHL	CHD-C1D	4.30	1.46	1.38
23	Au	609	CHL	C2C-C3C	4.30	1.46	1.36
23	9	606	CHL	CHC-C1C	4.30	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	605	CHL	CHD-C1D	4.30	1.46	1.38
23	Au	606	CHL	CHD-C1D	4.30	1.46	1.38
26	5	617	NEX	C34-C33	4.30	1.41	1.35
25	7	316	LUT	C34-C33	4.30	1.41	1.35
23	N	601	CHL	C2C-C3C	4.30	1.46	1.36
23	A2	601	CHL	C2C-C3C	4.30	1.46	1.36
26	G	617	NEX	C34-C33	4.30	1.41	1.35
28	BQ	619	XAT	C32-C33	4.30	1.55	1.45
23	A2	608	CHL	CHC-C1C	4.30	1.47	1.38
23	r	613	CHL	CHD-C1D	4.29	1.46	1.38
26	BV	616	NEX	C14-C13	4.29	1.41	1.35
28	g	619	XAT	C32-C33	4.29	1.55	1.45
23	BJ	601	CHL	CHC-C1C	4.29	1.47	1.38
23	S	606	CHL	CHC-C1C	4.29	1.47	1.38
23	Y	302	CHL	O2A-CGA	4.29	1.45	1.33
23	BQ	605	CHL	O2A-CGA	4.29	1.45	1.33
26	BJ	617	NEX	C34-C33	4.29	1.41	1.35
23	Y	310	CHL	CHC-C1C	4.29	1.47	1.38
23	A2	605	CHL	C2C-C3C	4.29	1.46	1.36
23	y	308	CHL	O2A-CGA	4.29	1.45	1.33
23	8	304	CHL	CHC-C1C	4.29	1.47	1.38
23	9	607	CHL	C2C-C3C	4.29	1.45	1.36
28	Y	301	XAT	C12-C13	4.29	1.55	1.45
28	BB	301	XAT	C12-C13	4.29	1.55	1.45
26	BQ	617	NEX	C14-C13	4.29	1.41	1.35
28	r	616	XAT	C12-C13	4.29	1.55	1.45
23	BU	605	CHL	O2A-CGA	4.28	1.45	1.33
28	y	301	XAT	C32-C33	4.28	1.55	1.45
23	AA	308	CHL	O2A-CGA	4.28	1.45	1.33
23	AB	306	CHL	O2A-CGA	4.28	1.45	1.30
23	AB	304	CHL	CHC-C1C	4.28	1.47	1.38
23	Y	309	CHL	C2C-C3C	4.28	1.45	1.36
23	AB	305	CHL	CHD-C1D	4.28	1.46	1.38
23	g	605	CHL	CHD-C1D	4.28	1.46	1.38
23	G	608	CHL	C2C-C3C	4.28	1.45	1.36
28	BU	616	XAT	C32-C33	4.28	1.55	1.45
23	7	307	CHL	CHD-C1D	4.28	1.46	1.38
23	AB	306	CHL	CHD-C1D	4.28	1.46	1.38
23	G	607	CHL	C2C-C3C	4.28	1.45	1.36
23	S	606	CHL	CHD-C1D	4.28	1.46	1.38
23	Au	607	CHL	CHC-C1C	4.28	1.47	1.38
23	s	606	CHL	CHD-C1D	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	608	CHL	C2C-C3C	4.28	1.45	1.36
23	Au	607	CHL	O2A-CGA	4.28	1.45	1.33
23	s	606	CHL	CHC-C1C	4.28	1.47	1.38
26	g	617	NEX	C34-C33	4.28	1.41	1.35
23	G	608	CHL	O2A-CGA	4.27	1.45	1.33
23	0	601	CHL	O2A-CGA	4.27	1.45	1.33
28	N	619	XAT	C32-C33	4.27	1.55	1.45
23	A2	608	CHL	CHD-C1D	4.27	1.46	1.38
23	A2	607	CHL	CHC-C1C	4.27	1.47	1.38
23	N	608	CHL	CHC-C1C	4.27	1.47	1.38
25	6	616	LUT	C10-C9	4.27	1.41	1.35
23	Y	306	CHL	CHD-C1D	4.27	1.46	1.38
23	Au	608	CHL	O2A-CGA	4.27	1.45	1.33
28	5	619	XAT	C12-C13	4.27	1.55	1.45
23	A6	605	CHL	CHC-C1C	4.27	1.47	1.38
26	Au	617	NEX	C14-C13	4.27	1.41	1.35
23	r	606	CHL	CHC-C1C	4.27	1.47	1.38
23	8	307	CHL	CHC-C1C	4.27	1.47	1.38
28	N	619	XAT	C12-C13	4.27	1.55	1.45
23	S	601	CHL	CHD-C1D	4.27	1.46	1.38
23	g	608	CHL	O2A-CGA	4.27	1.45	1.33
23	7	308	CHL	CHC-C1C	4.27	1.47	1.38
28	y	301	XAT	C12-C13	4.26	1.55	1.45
23	BJ	607	CHL	O2A-CGA	4.26	1.45	1.33
23	r	613	CHL	C2C-C3C	4.26	1.45	1.36
23	BB	309	CHL	C2C-C3C	4.26	1.45	1.36
26	7	319	NEX	C30-C29	4.26	1.41	1.35
23	BB	306	CHL	CHD-C1D	4.26	1.46	1.38
23	N	608	CHL	C2C-C3C	4.26	1.45	1.36
23	AB	305	CHL	CHC-C1C	4.26	1.47	1.38
31	2	404	PL9	C6-C1	-4.26	1.41	1.48
23	G	601	CHL	CHC-C1C	4.26	1.47	1.38
23	BJ	608	CHL	O2A-CGA	4.26	1.45	1.33
23	y	310	CHL	CHD-C4C	4.26	1.48	1.39
23	7	308	CHL	O2A-CGA	4.25	1.45	1.33
31	d	403	PL9	C3-C4	-4.25	1.42	1.49
23	6	607	CHL	CHD-C1D	4.25	1.46	1.38
23	8	306	CHL	O2A-CGA	4.25	1.45	1.30
23	A6	601	CHL	CHD-C1D	4.25	1.46	1.38
23	G	607	CHL	O2A-CGA	4.25	1.45	1.33
23	BU	613	CHL	C2C-C3C	4.25	1.45	1.36
25	6	616	LUT	C30-C29	4.25	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	608	CHL	CHD-C1D	4.25	1.46	1.38
25	5	616	LUT	C14-C13	4.25	1.41	1.35
23	N	609	CHL	CHC-C1C	4.25	1.47	1.38
23	AA	307	CHL	CHC-C1C	4.25	1.47	1.38
23	AA	308	CHL	CHC-C1C	4.25	1.47	1.38
23	0	601	CHL	C2C-C3C	4.25	1.45	1.36
23	BH	601	CHL	CHC-C1C	4.25	1.47	1.38
23	G	601	CHL	C2C-C3C	4.25	1.45	1.36
23	BU	607	CHL	O2A-CGA	4.25	1.45	1.33
23	S	601	CHL	C2C-C3C	4.25	1.45	1.36
23	8	305	CHL	CHC-C1C	4.25	1.47	1.38
23	0	607	CHL	O2A-CGA	4.24	1.45	1.33
23	BJ	601	CHL	CHD-C1D	4.24	1.46	1.38
23	A2	608	CHL	C2C-C3C	4.24	1.45	1.36
23	6	601	CHL	CHC-C1C	4.24	1.47	1.38
28	Ba	301	XAT	C32-C33	4.24	1.55	1.45
26	y	318	NEX	C14-C13	4.24	1.41	1.35
23	BQ	605	CHL	CHD-C1D	4.24	1.46	1.38
23	e	601	CHL	CHC-C1C	4.24	1.47	1.38
26	9	617	NEX	C34-C33	4.23	1.41	1.35
23	5	606	CHL	CHC-C1C	4.23	1.47	1.38
23	BJ	609	CHL	CHD-C4C	4.23	1.48	1.39
23	9	608	CHL	C2C-C3C	4.23	1.45	1.36
23	n	605	CHL	CHD-C1D	4.23	1.46	1.38
23	g	601	CHL	CHC-C1C	4.23	1.47	1.38
23	r	607	CHL	O2A-CGA	4.23	1.45	1.33
23	Y	310	CHL	C2C-C3C	4.23	1.45	1.36
23	N	607	CHL	CHC-C1C	4.23	1.47	1.38
28	BU	616	XAT	C12-C13	4.23	1.55	1.45
23	N	601	CHL	CHC-C1C	4.23	1.47	1.38
23	N	609	CHL	CHD-C1D	4.23	1.46	1.38
29	1	515	BCR	C30-C25	-4.23	1.48	1.53
23	5	607	CHL	CHD-C1D	4.23	1.46	1.38
23	A6	606	CHL	CHC-C1C	4.22	1.47	1.38
23	Ba	310	CHL	CHD-C4C	4.22	1.48	1.39
26	9	617	NEX	C14-C13	4.22	1.41	1.35
23	n	609	CHL	O2A-CGA	4.22	1.45	1.33
25	6	616	LUT	C34-C33	4.22	1.41	1.35
23	Au	609	CHL	O2A-CGA	4.22	1.45	1.33
23	A2	609	CHL	CHD-C1D	4.22	1.46	1.38
23	BQ	609	CHL	O2A-CGA	4.22	1.45	1.33
28	A2	619	XAT	C32-C33	4.22	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	607	CHL	O2A-CGA	4.22	1.45	1.33
31	BG	403	PL9	C7-C3	-4.22	1.47	1.51
23	Au	601	CHL	CHC-C1C	4.21	1.47	1.38
23	BJ	605	CHL	CHD-C1D	4.21	1.46	1.38
23	Ba	310	CHL	O2A-CGA	4.21	1.45	1.33
25	g	616	LUT	C30-C29	4.21	1.41	1.35
23	g	609	CHL	CHD-C4C	4.21	1.48	1.39
25	BJ	616	LUT	C30-C29	4.21	1.41	1.35
23	8	305	CHL	CHD-C1D	4.21	1.46	1.38
23	A6	606	CHL	CHD-C1D	4.21	1.46	1.38
23	BV	606	CHL	CHD-C1D	4.21	1.46	1.38
25	BB	317	LUT	C34-C33	4.21	1.41	1.35
23	G	609	CHL	C2C-C3C	4.21	1.45	1.36
23	5	601	CHL	CHD-C1D	4.21	1.46	1.38
23	5	608	CHL	CHC-C1C	4.21	1.47	1.38
23	BB	302	CHL	O2A-CGA	4.21	1.45	1.33
28	A2	619	XAT	C12-C13	4.21	1.55	1.45
23	0	609	CHL	C2C-C3C	4.21	1.45	1.36
29	R	410	BCR	C1-C6	-4.21	1.48	1.53
26	g	617	NEX	C30-C29	4.20	1.41	1.35
23	G	609	CHL	O2A-CGA	4.20	1.45	1.33
23	AA	309	CHL	CHC-C1C	4.20	1.47	1.38
25	9	615	LUT	C34-C33	4.20	1.41	1.35
25	BQ	615	LUT	C10-C9	4.20	1.41	1.35
23	A2	601	CHL	CHD-C1D	4.20	1.46	1.38
23	7	307	CHL	CHC-C1C	4.20	1.47	1.38
23	N	606	CHL	C2C-C3C	4.20	1.45	1.36
26	s	616	NEX	C14-C13	4.20	1.41	1.35
23	Au	607	CHL	C2C-C3C	4.20	1.45	1.36
23	AA	306	CHL	CHD-C4C	4.20	1.48	1.39
23	BQ	608	CHL	O2A-CGA	4.20	1.45	1.33
23	0	601	CHL	CHC-C1C	4.20	1.47	1.38
23	N	601	CHL	CHD-C1D	4.20	1.46	1.38
23	n	608	CHL	O2A-CGA	4.20	1.45	1.33
23	A2	601	CHL	CHC-C1C	4.20	1.47	1.38
23	N	605	CHL	CHD-C1D	4.19	1.46	1.38
23	A2	609	CHL	CHC-C1C	4.19	1.47	1.38
23	BB	310	CHL	CHC-C1C	4.19	1.47	1.38
23	Au	608	CHL	C2C-C3C	4.19	1.45	1.36
26	BB	320	NEX	C14-C13	4.19	1.41	1.35
23	A2	605	CHL	CHD-C1D	4.19	1.46	1.38
23	A2	607	CHL	C2C-C3C	4.19	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	307	CHL	CHC-C1C	4.19	1.47	1.38
25	5	615	LUT	C10-C9	4.19	1.41	1.35
23	7	309	CHL	CHC-C1C	4.19	1.47	1.38
23	g	608	CHL	CHC-C1C	4.19	1.47	1.38
26	y	318	NEX	C30-C29	4.19	1.41	1.35
23	N	606	CHL	CHD-C1D	4.19	1.46	1.38
23	BU	606	CHL	CHD-C1D	4.18	1.46	1.38
23	y	310	CHL	O2A-CGA	4.18	1.45	1.33
23	N	605	CHL	O2A-CGA	4.18	1.45	1.33
23	A2	606	CHL	C2C-C3C	4.18	1.45	1.36
26	BQ	617	NEX	C30-C29	4.18	1.41	1.35
26	BJ	617	NEX	C30-C29	4.18	1.41	1.35
23	A2	606	CHL	CHD-C1D	4.18	1.46	1.38
25	0	616	LUT	C10-C9	4.17	1.41	1.35
23	5	609	CHL	CHD-C4C	4.17	1.48	1.39
26	5	617	NEX	C14-C13	4.17	1.41	1.35
23	9	609	CHL	C2C-C3C	4.17	1.45	1.36
23	7	306	CHL	CHD-C4C	4.17	1.48	1.39
23	9	608	CHL	CHC-C1C	4.17	1.47	1.38
23	5	608	CHL	CHD-C1D	4.17	1.46	1.38
23	Y	302	CHL	CHC-C1C	4.17	1.47	1.38
23	S	605	CHL	C2C-C3C	4.17	1.45	1.36
25	n	615	LUT	C10-C9	4.17	1.41	1.35
23	G	609	CHL	CHD-C4C	4.17	1.48	1.39
23	5	609	CHL	O2A-CGA	4.16	1.45	1.33
23	A2	605	CHL	O2A-CGA	4.16	1.45	1.33
23	0	609	CHL	O2A-CGA	4.16	1.45	1.33
23	y	306	CHL	O2A-CGA	4.16	1.45	1.33
23	N	607	CHL	C2C-C3C	4.16	1.45	1.36
23	y	309	CHL	O2A-CGA	4.16	1.45	1.33
23	Y	309	CHL	CHD-C1D	4.16	1.46	1.38
23	BB	309	CHL	CHD-C1D	4.16	1.46	1.38
23	A6	601	CHL	C2C-C3C	4.16	1.45	1.36
23	Y	302	CHL	CHD-C1D	4.15	1.46	1.38
25	n	615	LUT	C14-C13	4.15	1.41	1.35
23	Ba	309	CHL	O2A-CGA	4.15	1.45	1.33
23	BU	613	CHL	CHC-C1C	4.15	1.47	1.38
23	Y	307	CHL	CHC-C1C	4.15	1.46	1.38
23	9	609	CHL	O2A-CGA	4.15	1.45	1.33
26	n	617	NEX	C30-C29	4.15	1.41	1.35
23	6	608	CHL	C2C-C3C	4.15	1.45	1.36
23	7	310	CHL	CHD-C4C	4.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	606	CHL	CHD-C1D	4.15	1.46	1.38
23	BJ	608	CHL	CHC-C1C	4.15	1.46	1.38
23	9	608	CHL	CHD-C1D	4.15	1.46	1.38
26	BQ	617	NEX	C34-C33	4.14	1.41	1.35
23	9	601	CHL	CHD-C1D	4.14	1.46	1.38
29	BN	101	BCR	C1-C6	-4.14	1.48	1.53
23	G	601	CHL	CHD-C1D	4.14	1.46	1.38
23	Y	306	CHL	O2A-CGA	4.14	1.45	1.33
25	BJ	616	LUT	C34-C33	4.14	1.41	1.35
26	Ba	318	NEX	C14-C13	4.14	1.41	1.35
23	r	607	CHL	CHD-C1D	4.14	1.46	1.38
23	S	605	CHL	CHD-C1D	4.14	1.46	1.38
25	6	616	LUT	C14-C13	4.14	1.41	1.35
23	0	608	CHL	C2C-C3C	4.14	1.45	1.36
25	g	616	LUT	C34-C33	4.14	1.41	1.35
23	Ba	306	CHL	O2A-CGA	4.14	1.45	1.33
23	BB	306	CHL	O2A-CGA	4.14	1.45	1.33
23	s	607	CHL	CHD-C4C	4.14	1.48	1.39
23	r	613	CHL	CHC-C1C	4.14	1.46	1.38
26	r	617	NEX	C14-C13	4.13	1.41	1.35
23	Au	609	CHL	CHD-C1D	4.13	1.46	1.38
29	A	411	BCR	C1-C6	-4.13	1.48	1.53
23	A2	609	CHL	C2C-C3C	4.13	1.45	1.36
23	N	608	CHL	O2A-CGA	4.13	1.45	1.33
23	BJ	609	CHL	O2A-CGA	4.13	1.45	1.33
25	9	615	LUT	C14-C13	4.13	1.41	1.35
23	9	609	CHL	CHC-C4B	4.13	1.48	1.39
23	5	607	CHL	CHC-C1C	4.13	1.46	1.38
23	N	605	CHL	CHC-C1C	4.13	1.46	1.38
26	G	617	NEX	C30-C29	4.13	1.41	1.35
26	n	617	NEX	C34-C33	4.12	1.41	1.35
28	9	619	XAT	C32-C33	4.12	1.54	1.45
25	N	615	LUT	C34-C33	4.12	1.41	1.35
23	7	310	CHL	O2A-CGA	4.12	1.45	1.33
23	G	607	CHL	CHD-C1D	4.12	1.46	1.38
29	AB	313	BCR	C1-C6	-4.12	1.48	1.53
26	AA	319	NEX	C34-C33	4.12	1.41	1.35
23	N	609	CHL	C2C-C3C	4.12	1.45	1.36
23	6	609	CHL	O2A-CGA	4.12	1.45	1.33
25	5	616	LUT	C30-C29	4.12	1.41	1.35
25	0	615	LUT	C14-C13	4.12	1.41	1.35
25	BQ	616	LUT	C10-C9	4.12	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BU	607	CHL	CHD-C1D	4.12	1.46	1.38
23	A2	608	CHL	O2A-CGA	4.12	1.45	1.33
23	BB	309	CHL	O2A-CGA	4.12	1.45	1.33
23	6	606	CHL	C2C-C3C	4.12	1.45	1.36
23	BB	310	CHL	C2C-C3C	4.12	1.45	1.36
23	BB	302	CHL	CHC-C1C	4.12	1.46	1.38
23	A6	607	CHL	CHD-C4C	4.12	1.48	1.39
23	5	607	CHL	O2A-CGA	4.11	1.45	1.33
25	A2	615	LUT	C34-C33	4.11	1.41	1.35
23	BB	302	CHL	CHD-C1D	4.11	1.46	1.38
23	g	609	CHL	O2A-CGA	4.11	1.45	1.33
25	Y	317	LUT	C34-C33	4.11	1.41	1.35
23	Y	309	CHL	O2A-CGA	4.11	1.45	1.33
23	A6	605	CHL	CHD-C1D	4.11	1.46	1.38
25	BQ	615	LUT	C14-C13	4.11	1.41	1.35
26	Ba	318	NEX	C30-C29	4.10	1.41	1.35
23	AA	310	CHL	O2A-CGA	4.09	1.45	1.33
23	Au	607	CHL	CHD-C1D	4.09	1.46	1.38
23	AA	310	CHL	CHD-C4C	4.09	1.48	1.39
25	0	616	LUT	C30-C29	4.09	1.41	1.35
23	9	607	CHL	O2A-CGA	4.09	1.45	1.33
26	BV	616	NEX	C30-C29	4.09	1.41	1.35
25	BQ	616	LUT	C34-C33	4.09	1.41	1.35
23	A6	605	CHL	C2C-C3C	4.09	1.45	1.36
23	BH	601	CHL	CHD-C1D	4.09	1.46	1.38
25	7	317	LUT	C10-C9	4.08	1.41	1.35
25	0	616	LUT	C14-C13	4.08	1.41	1.35
26	A6	616	NEX	C14-C13	4.08	1.41	1.35
26	BV	616	NEX	C34-C33	4.08	1.41	1.35
25	AA	316	LUT	C14-C13	4.08	1.41	1.35
23	Au	601	CHL	CHD-C1D	4.08	1.46	1.38
23	Au	601	CHL	C2C-C3C	4.08	1.45	1.36
23	9	607	CHL	CHC-C1C	4.08	1.46	1.38
23	BV	607	CHL	CHD-C4C	4.08	1.48	1.39
26	A6	616	NEX	C34-C33	4.08	1.41	1.35
28	5	619	XAT	C32-C33	4.07	1.54	1.45
25	BQ	616	LUT	C14-C13	4.07	1.41	1.35
23	BB	308	CHL	CHC-C1C	4.07	1.46	1.38
25	9	616	LUT	C14-C13	4.07	1.41	1.35
23	y	309	CHL	CHD-C4C	4.06	1.48	1.39
23	9	607	CHL	CHD-C1D	4.06	1.46	1.38
26	Au	617	NEX	C30-C29	4.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BV	614	LUT	C30-C29	4.06	1.41	1.35
23	Ba	309	CHL	CHD-C4C	4.06	1.48	1.39
23	N	607	CHL	CHD-C1D	4.06	1.46	1.38
23	e	601	CHL	CHD-C1D	4.05	1.46	1.38
23	Ba	310	CHL	CHC-C4B	4.05	1.48	1.39
23	A2	607	CHL	CHD-C1D	4.05	1.46	1.38
29	C	515	BCR	C30-C25	-4.05	1.48	1.53
23	7	308	CHL	CHD-C1D	4.05	1.46	1.38
23	0	606	CHL	C2C-C3C	4.05	1.45	1.36
28	8	312	XAT	C12-C13	4.04	1.54	1.45
23	AA	308	CHL	CHD-C1D	4.04	1.46	1.38
23	A2	605	CHL	CHC-C1C	4.04	1.46	1.38
26	s	616	NEX	C30-C29	4.04	1.41	1.35
26	7	319	NEX	C34-C33	4.03	1.41	1.35
29	BF	515	BCR	C1-C6	-4.03	1.48	1.53
23	6	607	CHL	CHC-C1C	4.03	1.46	1.38
26	S	616	NEX	C14-C13	4.03	1.41	1.35
23	Au	605	CHL	CHD-C4C	4.03	1.48	1.39
29	c	515	BCR	C30-C25	-4.03	1.48	1.53
26	y	318	NEX	C34-C33	4.03	1.41	1.35
25	Au	615	LUT	C34-C33	4.03	1.41	1.35
23	Y	307	CHL	C2C-C3C	4.02	1.45	1.36
26	s	616	NEX	C34-C33	4.02	1.41	1.35
25	BQ	615	LUT	C30-C29	4.02	1.41	1.35
25	7	317	LUT	C34-C33	4.02	1.41	1.35
23	AA	302	CHL	CHD-C4C	4.02	1.48	1.39
23	Y	308	CHL	CHC-C1C	4.01	1.46	1.38
25	n	615	LUT	C30-C29	4.01	1.41	1.35
23	Y	308	CHL	C2C-C3C	4.01	1.45	1.36
26	r	617	NEX	C34-C33	4.01	1.41	1.35
25	0	615	LUT	C34-C33	4.01	1.41	1.35
25	S	614	LUT	C34-C33	4.00	1.41	1.35
23	BB	308	CHL	C2C-C3C	4.00	1.45	1.36
23	r	607	CHL	CHC-C1C	4.00	1.46	1.38
25	9	616	LUT	C34-C33	4.00	1.41	1.35
23	BU	607	CHL	CHC-C1C	4.00	1.46	1.38
23	y	310	CHL	CHC-C4B	4.00	1.48	1.39
29	1	515	BCR	C1-C6	-4.00	1.48	1.53
25	9	615	LUT	C10-C9	4.00	1.41	1.35
28	AB	312	XAT	C12-C13	4.00	1.54	1.45
23	G	608	CHL	CHD-C4C	4.00	1.48	1.39
25	n	615	LUT	C34-C33	4.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	318	NEX	C14-C13	4.00	1.41	1.35
23	s	605	CHL	CHD-C4C	3.99	1.48	1.39
23	7	302	CHL	CHD-C4C	3.99	1.48	1.39
23	y	302	CHL	CHD-C4C	3.99	1.48	1.39
26	BB	320	NEX	C34-C33	3.99	1.41	1.35
23	S	607	CHL	CHD-C1D	3.99	1.46	1.38
25	BV	614	LUT	C34-C33	3.99	1.41	1.35
25	n	616	LUT	C34-C33	3.99	1.41	1.35
23	6	606	CHL	CHD-C1D	3.98	1.46	1.38
25	AA	316	LUT	C34-C33	3.98	1.41	1.35
25	A6	614	LUT	C34-C33	3.98	1.41	1.35
23	Y	302	CHL	C2C-C3C	3.98	1.45	1.36
26	S	616	NEX	C34-C33	3.98	1.41	1.35
29	C	515	BCR	C1-C6	-3.98	1.48	1.53
25	G	615	LUT	C10-C9	3.98	1.41	1.35
23	n	608	CHL	CHD-C4C	3.97	1.48	1.39
26	S	616	NEX	C30-C29	3.97	1.41	1.35
29	8	313	BCR	C1-C6	-3.97	1.48	1.53
29	4	101	BCR	C1-C6	-3.97	1.48	1.53
25	y	317	LUT	C14-C13	3.97	1.41	1.35
25	N	615	LUT	C10-C9	3.97	1.41	1.35
23	0	609	CHL	CHC-C4B	3.97	1.48	1.39
23	AA	309	CHL	CHD-C4C	3.97	1.48	1.39
25	S	614	LUT	C10-C9	3.97	1.41	1.35
23	Ba	302	CHL	CHD-C4C	3.96	1.48	1.39
26	n	617	NEX	C14-C13	3.96	1.41	1.35
23	6	605	CHL	CHD-C4C	3.96	1.48	1.39
25	AA	317	LUT	C10-C9	3.96	1.41	1.35
23	G	605	CHL	CHD-C4C	3.96	1.48	1.39
29	Bb	101	BCR	C1-C6	-3.95	1.48	1.53
26	A6	616	NEX	C30-C29	3.95	1.41	1.35
23	0	606	CHL	CHD-C1D	3.95	1.46	1.38
25	G	616	LUT	C34-C33	3.95	1.41	1.35
31	d	403	PL9	C7-C3	-3.95	1.47	1.51
23	n	601	CHL	CHD-C4C	3.95	1.48	1.39
23	BQ	606	CHL	CHD-C4C	3.95	1.48	1.39
23	Au	608	CHL	CHD-C4C	3.95	1.48	1.39
25	s	615	LUT	C14-C13	3.95	1.41	1.35
26	Y	318	NEX	C14-C13	3.95	1.41	1.35
25	Au	615	LUT	C10-C9	3.95	1.41	1.35
23	BQ	609	CHL	CHD-C4C	3.95	1.48	1.39
25	G	615	LUT	C34-C33	3.95	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AA	301	XAT	C31-C30	3.95	1.55	1.43
23	Y	307	CHL	CHD-C1D	3.94	1.46	1.38
23	BU	605	CHL	CHD-C1D	3.94	1.46	1.38
23	Ba	308	CHL	CHD-C4C	3.94	1.48	1.39
25	BV	615	LUT	C14-C13	3.94	1.41	1.35
26	Ba	318	NEX	C34-C33	3.94	1.41	1.35
25	BV	615	LUT	C34-C33	3.94	1.41	1.35
23	BJ	608	CHL	CHD-C4C	3.94	1.48	1.39
25	N	616	LUT	C14-C13	3.94	1.41	1.35
23	r	605	CHL	CHD-C1D	3.94	1.46	1.38
24	g	611	CLA	C1D-ND	3.94	1.42	1.37
23	BV	601	CHL	CHD-C4C	3.93	1.48	1.39
23	Au	609	CHL	CHC-C1C	3.93	1.46	1.38
23	8	306	CHL	CHD-C4C	3.93	1.48	1.39
23	s	601	CHL	CHD-C4C	3.93	1.48	1.39
23	BQ	601	CHL	CHD-C4C	3.93	1.48	1.39
23	AB	306	CHL	CHD-C4C	3.93	1.48	1.39
29	BD	411	BCR	C1-C6	-3.93	1.48	1.53
23	7	309	CHL	CHD-C4C	3.93	1.48	1.39
23	6	606	CHL	CHC-C1C	3.93	1.46	1.38
25	5	615	LUT	C30-C29	3.93	1.41	1.35
23	BV	605	CHL	CHD-C4C	3.93	1.48	1.39
23	0	607	CHL	CHC-C1C	3.93	1.46	1.38
25	S	615	LUT	C30-C29	3.93	1.41	1.35
25	BQ	615	LUT	C34-C33	3.93	1.41	1.35
25	Ba	317	LUT	C14-C13	3.93	1.41	1.35
24	s	603	CLA	C1D-ND	3.93	1.42	1.37
24	BJ	611	CLA	C1D-ND	3.93	1.42	1.37
25	Au	616	LUT	C10-C9	3.92	1.41	1.35
23	n	607	CHL	CHD-C4C	3.92	1.48	1.39
23	g	607	CHL	CHD-C4C	3.92	1.48	1.39
23	BQ	608	CHL	CHD-C4C	3.92	1.48	1.39
23	AB	307	CHL	CHD-C4C	3.92	1.48	1.39
25	Y	316	LUT	C34-C33	3.92	1.41	1.35
26	A2	617	NEX	C14-C13	3.92	1.41	1.35
23	8	307	CHL	CHD-C4C	3.91	1.48	1.39
23	n	609	CHL	CHD-C4C	3.91	1.48	1.39
23	y	308	CHL	CHD-C4C	3.91	1.48	1.39
23	0	606	CHL	CHC-C1C	3.91	1.46	1.38
23	g	608	CHL	CHD-C4C	3.91	1.48	1.39
25	A6	614	LUT	C10-C9	3.91	1.41	1.35
26	S	616	NEX	C10-C9	3.91	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	0	605	CHL	CHD-C4C	3.91	1.48	1.39
25	Y	316	LUT	C30-C29	3.91	1.41	1.35
23	Y	310	CHL	CHD-C4C	3.91	1.48	1.39
25	N	615	LUT	C30-C29	3.91	1.41	1.35
25	A2	615	LUT	C30-C29	3.91	1.41	1.35
25	BB	316	LUT	C34-C33	3.91	1.41	1.35
29	z	101	BCR	C1-C6	-3.91	1.48	1.53
23	y	306	CHL	CHD-C4C	3.91	1.48	1.39
23	BB	307	CHL	CHD-C1D	3.91	1.46	1.38
25	s	615	LUT	C34-C33	3.91	1.41	1.35
25	BB	316	LUT	C30-C29	3.91	1.41	1.35
25	A6	615	LUT	C30-C29	3.91	1.41	1.35
38	A	408	PHO	C1D-C2D	3.90	1.43	1.39
28	7	301	XAT	C31-C30	3.90	1.55	1.43
23	BB	307	CHL	C2C-C3C	3.90	1.45	1.36
23	BQ	607	CHL	CHD-C4C	3.90	1.48	1.39
23	9	601	CHL	CHD-C4C	3.90	1.48	1.39
23	BJ	606	CHL	CHD-C4C	3.90	1.48	1.39
28	8	312	XAT	C11-C10	3.90	1.55	1.43
23	n	606	CHL	CHD-C4C	3.90	1.48	1.39
29	C	514	BCR	C1-C6	-3.90	1.48	1.53
23	0	607	CHL	CHD-C4C	3.90	1.48	1.39
28	AB	312	XAT	C11-C10	3.90	1.55	1.43
25	s	614	LUT	C30-C29	3.90	1.40	1.35
23	g	606	CHL	CHD-C4C	3.90	1.48	1.39
23	5	601	CHL	CHD-C4C	3.89	1.48	1.39
23	BU	613	CHL	CHD-C4C	3.89	1.48	1.39
25	s	614	LUT	C10-C9	3.89	1.40	1.35
23	BJ	607	CHL	CHD-C4C	3.89	1.48	1.39
23	S	601	CHL	CHD-C4C	3.89	1.48	1.39
29	F	101	BCR	C1-C6	-3.89	1.48	1.53
25	g	615	LUT	C14-C13	3.89	1.40	1.35
25	BV	614	LUT	C10-C9	3.89	1.40	1.35
24	g	604	CLA	C1D-ND	3.89	1.42	1.37
25	9	616	LUT	C30-C29	3.89	1.40	1.35
23	Ba	306	CHL	CHD-C4C	3.89	1.48	1.39
23	Y	306	CHL	CHD-C4C	3.89	1.48	1.39
23	S	606	CHL	CHD-C4C	3.88	1.48	1.39
24	BJ	604	CLA	C1D-ND	3.88	1.42	1.37
23	5	605	CHL	CHD-C4C	3.88	1.48	1.39
25	Au	616	LUT	C34-C33	3.88	1.40	1.35
23	y	309	CHL	OBD-CAD	3.88	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	304	CHL	CHD-C4C	3.88	1.48	1.39
23	BB	308	CHL	CHD-C1D	3.88	1.45	1.38
25	Au	615	LUT	C30-C29	3.88	1.40	1.35
25	S	615	LUT	C14-C13	3.88	1.40	1.35
23	6	601	CHL	CHD-C4C	3.87	1.48	1.39
23	9	605	CHL	CHD-C4C	3.87	1.48	1.39
23	BU	605	CHL	CHD-C4C	3.87	1.48	1.39
23	r	613	CHL	CHD-C4C	3.87	1.48	1.39
23	0	601	CHL	CHD-C4C	3.87	1.48	1.39
23	BJ	601	CHL	CHD-C4C	3.87	1.48	1.39
23	BV	606	CHL	CHD-C4C	3.87	1.48	1.39
23	BB	302	CHL	C2C-C3C	3.87	1.45	1.36
25	0	615	LUT	C10-C9	3.87	1.40	1.35
25	n	616	LUT	C10-C9	3.87	1.40	1.35
25	A2	616	LUT	C14-C13	3.87	1.40	1.35
23	A2	601	CHL	CHD-C4C	3.87	1.48	1.39
23	g	601	CHL	CHD-C4C	3.87	1.48	1.39
23	g	605	CHL	CHD-C4C	3.87	1.48	1.39
23	N	601	CHL	CHD-C4C	3.87	1.48	1.39
24	BV	603	CLA	C1D-ND	3.86	1.42	1.37
28	Au	619	XAT	C31-C30	3.86	1.55	1.43
29	1	514	BCR	C30-C25	-3.86	1.48	1.53
25	BV	614	LUT	C14-C13	3.86	1.40	1.35
23	r	605	CHL	CHD-C4C	3.86	1.48	1.39
23	Y	308	CHL	CHD-C1D	3.86	1.45	1.38
28	AA	301	XAT	C11-C10	3.86	1.55	1.43
25	s	614	LUT	C34-C33	3.86	1.40	1.35
23	A6	601	CHL	CHD-C4C	3.86	1.48	1.39
24	g	610	CLA	C1D-ND	3.86	1.42	1.37
25	G	615	LUT	C30-C29	3.86	1.40	1.35
29	B	623	BCR	C1-C6	-3.86	1.48	1.53
28	G	619	XAT	C31-C30	3.86	1.55	1.43
25	BJ	615	LUT	C14-C13	3.86	1.40	1.35
28	BJ	619	XAT	C11-C10	3.85	1.55	1.43
25	A6	615	LUT	C14-C13	3.85	1.40	1.35
23	8	305	CHL	CHD-C4C	3.85	1.48	1.39
23	BJ	605	CHL	CHD-C4C	3.85	1.48	1.39
25	s	615	LUT	C10-C9	3.85	1.40	1.35
23	6	608	CHL	CHD-C4C	3.85	1.48	1.39
23	A6	606	CHL	CHD-C4C	3.85	1.48	1.39
23	AB	304	CHL	CHD-C4C	3.85	1.48	1.39
25	BV	615	LUT	C30-C29	3.85	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BJ	612	CLA	C1D-ND	3.85	1.42	1.37
29	z	102	BCR	C1-C6	-3.85	1.48	1.53
24	g	614	CLA	C1D-ND	3.85	1.42	1.37
23	s	606	CHL	CHD-C4C	3.85	1.48	1.39
29	a	411	BCR	C1-C6	-3.85	1.48	1.53
28	g	619	XAT	C11-C10	3.85	1.55	1.43
29	k	101	BCR	C1-C6	-3.85	1.48	1.53
25	5	616	LUT	C10-C9	3.85	1.40	1.35
25	BV	615	LUT	C10-C9	3.85	1.40	1.35
28	Y	301	XAT	C15-C14	3.84	1.55	1.43
25	BQ	616	LUT	C30-C29	3.84	1.40	1.35
25	n	616	LUT	C30-C29	3.84	1.40	1.35
24	s	604	CLA	C1D-ND	3.84	1.42	1.37
25	9	616	LUT	C10-C9	3.84	1.40	1.35
25	S	614	LUT	C14-C13	3.84	1.40	1.35
28	Y	301	XAT	C31-C30	3.84	1.55	1.43
32	L	101	SQD	O47-C45	-3.84	1.37	1.46
24	BJ	614	CLA	C1D-ND	3.84	1.42	1.37
28	n	619	XAT	C11-C10	3.84	1.55	1.43
32	Az	101	SQD	O47-C45	-3.84	1.37	1.46
28	7	301	XAT	C11-C10	3.84	1.55	1.43
25	Ba	317	LUT	C34-C33	3.83	1.40	1.35
28	G	619	XAT	C11-C10	3.83	1.55	1.43
28	BB	301	XAT	C15-C14	3.83	1.55	1.43
25	s	614	LUT	C14-C13	3.83	1.40	1.35
24	g	612	CLA	C1D-ND	3.83	1.42	1.37
25	S	614	LUT	C30-C29	3.83	1.40	1.35
25	A6	614	LUT	C30-C29	3.83	1.40	1.35
25	y	317	LUT	C34-C33	3.83	1.40	1.35
29	BF	516	BCR	C1-C6	-3.83	1.48	1.53
28	Au	619	XAT	C15-C14	3.82	1.55	1.43
25	A2	615	LUT	C10-C9	3.82	1.40	1.35
28	G	619	XAT	C15-C14	3.82	1.55	1.43
23	6	607	CHL	CHD-C4C	3.82	1.48	1.39
25	s	615	LUT	C30-C29	3.82	1.40	1.35
23	g	609	CHL	CHC-C4B	3.82	1.48	1.39
28	G	619	XAT	C35-C34	3.82	1.55	1.43
29	K	102	BCR	C1-C6	-3.82	1.48	1.53
23	BQ	609	CHL	CHC-C4B	3.82	1.48	1.39
25	g	616	LUT	C10-C9	3.82	1.40	1.35
25	9	615	LUT	C30-C29	3.82	1.40	1.35
24	BJ	610	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BV	604	CLA	C1D-ND	3.82	1.42	1.37
23	AB	305	CHL	CHD-C4C	3.82	1.47	1.39
25	G	616	LUT	C10-C9	3.82	1.40	1.35
28	A2	619	XAT	C31-C30	3.81	1.55	1.43
23	0	608	CHL	CHD-C4C	3.81	1.47	1.39
31	BG	403	PL9	C6-C1	-3.81	1.41	1.48
28	Au	619	XAT	C11-C10	3.81	1.55	1.43
23	Au	601	CHL	CHD-C4C	3.81	1.47	1.39
28	AA	301	XAT	C15-C14	3.81	1.55	1.43
28	Au	619	XAT	C35-C34	3.81	1.55	1.43
26	Y	318	NEX	C34-C33	3.81	1.40	1.35
29	AB	313	BCR	C30-C25	-3.81	1.48	1.53
28	BU	616	XAT	C11-C10	3.81	1.55	1.43
28	7	301	XAT	C15-C14	3.81	1.55	1.43
23	Ba	309	CHL	OBD-CAD	3.81	1.29	1.22
29	BE	618	BCR	C1-C6	-3.81	1.48	1.53
23	BB	306	CHL	CHD-C4C	3.81	1.47	1.39
24	BV	611	CLA	C1D-ND	3.81	1.42	1.37
23	5	608	CHL	CHD-C4C	3.81	1.47	1.39
28	AB	312	XAT	C31-C30	3.81	1.55	1.43
28	AA	318	XAT	C11-C10	3.81	1.55	1.43
28	7	318	XAT	C11-C10	3.81	1.55	1.43
28	BB	301	XAT	C31-C30	3.81	1.55	1.43
28	7	301	XAT	C35-C34	3.80	1.55	1.43
23	BJ	609	CHL	CHC-C4B	3.80	1.47	1.39
28	N	619	XAT	C15-C14	3.80	1.55	1.43
23	7	306	CHL	OBD-CAD	3.80	1.29	1.22
24	n	614	CLA	C1D-ND	3.80	1.42	1.37
24	BQ	614	CLA	C1D-ND	3.80	1.42	1.37
23	s	601	CHL	CHC-C4B	3.80	1.47	1.39
28	BQ	619	XAT	C11-C10	3.80	1.55	1.43
24	N	614	CLA	C1D-ND	3.80	1.42	1.37
23	Y	302	CHL	CHD-C4C	3.80	1.47	1.39
28	8	312	XAT	C31-C30	3.80	1.55	1.43
28	g	619	XAT	C31-C30	3.79	1.55	1.43
25	A6	614	LUT	C14-C13	3.79	1.40	1.35
23	N	608	CHL	CHD-C4C	3.79	1.47	1.39
23	BH	601	CHL	CHD-C4C	3.79	1.47	1.39
25	A6	615	LUT	C34-C33	3.79	1.40	1.35
29	v	622	BCR	C1-C6	-3.79	1.48	1.53
24	9	614	CLA	C1D-ND	3.79	1.42	1.37
23	Au	606	CHL	CHD-C4C	3.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	302	CHL	CHC-C4B	3.79	1.47	1.39
23	BB	310	CHL	CHD-C4C	3.79	1.47	1.39
28	9	619	XAT	C15-C14	3.79	1.55	1.43
28	Y	301	XAT	C11-C10	3.79	1.55	1.43
23	g	608	CHL	OBD-CAD	3.79	1.29	1.22
23	BJ	608	CHL	OBD-CAD	3.79	1.29	1.22
24	g	613	CLA	C1D-ND	3.79	1.42	1.37
28	AA	301	XAT	C35-C34	3.79	1.55	1.43
23	e	601	CHL	CHD-C4C	3.79	1.47	1.39
25	AA	316	LUT	C30-C29	3.79	1.40	1.35
25	BJ	615	LUT	C10-C9	3.79	1.40	1.35
28	r	616	XAT	C11-C10	3.79	1.55	1.43
23	Au	609	CHL	CHD-C4C	3.79	1.47	1.39
28	n	619	XAT	C31-C30	3.79	1.55	1.43
23	n	605	CHL	CHD-C4C	3.79	1.47	1.39
23	Y	309	CHL	CHD-C4C	3.79	1.47	1.39
28	N	619	XAT	C31-C30	3.79	1.55	1.43
24	n	613	CLA	C1D-ND	3.79	1.42	1.37
29	BF	515	BCR	C30-C25	-3.79	1.48	1.53
23	BV	601	CHL	CHC-C4B	3.79	1.47	1.39
38	a	408	PHO	C1D-C2D	3.79	1.43	1.39
23	G	606	CHL	CHD-C4C	3.79	1.47	1.39
23	S	605	CHL	CHD-C4C	3.79	1.47	1.39
23	BB	309	CHL	CHD-C4C	3.78	1.47	1.39
23	9	608	CHL	CHD-C4C	3.78	1.47	1.39
23	G	605	CHL	OBD-CAD	3.78	1.29	1.22
28	A2	619	XAT	C15-C14	3.78	1.55	1.43
23	A6	607	CHL	CHC-C4B	3.78	1.47	1.39
28	g	619	XAT	C35-C34	3.78	1.55	1.43
23	BV	607	CHL	OBD-CAD	3.78	1.29	1.22
24	AA	315	CLA	C1D-ND	3.78	1.42	1.37
25	Ba	316	LUT	C34-C33	3.78	1.40	1.35
28	N	619	XAT	C35-C34	3.78	1.55	1.43
24	A2	614	CLA	C1D-ND	3.78	1.42	1.37
28	g	619	XAT	C15-C14	3.78	1.55	1.43
23	AA	306	CHL	OBD-CAD	3.78	1.29	1.22
23	G	601	CHL	CHD-C4C	3.78	1.47	1.39
29	K	101	BCR	C1-C6	-3.78	1.48	1.53
23	Au	605	CHL	OBD-CAD	3.78	1.29	1.22
23	BQ	601	CHL	OBD-CAD	3.77	1.29	1.22
28	BJ	619	XAT	C31-C30	3.77	1.55	1.43
28	9	619	XAT	C11-C10	3.77	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A2	619	XAT	C35-C34	3.77	1.55	1.43
26	BB	318	NEX	C34-C33	3.77	1.40	1.35
23	AA	302	CHL	CHC-C4B	3.77	1.47	1.39
32	BO	102	SQD	O47-C45	-3.77	1.37	1.46
23	AA	307	CHL	CHD-C4C	3.77	1.47	1.39
23	5	607	CHL	CHD-C4C	3.77	1.47	1.39
23	7	307	CHL	CHD-C4C	3.77	1.47	1.39
23	Ba	310	CHL	CHB-C1B	3.77	1.47	1.39
24	BV	609	CLA	C1D-ND	3.77	1.42	1.37
25	S	615	LUT	C34-C33	3.77	1.40	1.35
29	1	514	BCR	C1-C6	-3.77	1.48	1.53
25	N	616	LUT	C34-C33	3.77	1.40	1.35
28	Y	301	XAT	C35-C34	3.77	1.55	1.43
28	BB	301	XAT	C11-C10	3.77	1.55	1.43
29	8	313	BCR	C30-C25	-3.77	1.48	1.53
23	S	607	CHL	CHC-C4B	3.77	1.47	1.39
29	C	514	BCR	C30-C25	-3.77	1.48	1.53
23	g	607	CHL	OBD-CAD	3.76	1.29	1.22
25	Ba	317	LUT	C10-C9	3.76	1.40	1.35
23	Ba	310	CHL	OBD-CAD	3.76	1.29	1.22
25	Ba	316	LUT	C14-C13	3.76	1.40	1.35
23	6	609	CHL	CHC-C4B	3.76	1.47	1.39
23	BB	302	CHL	CHD-C4C	3.76	1.47	1.39
24	r	614	CLA	C1D-ND	3.76	1.42	1.37
24	5	614	CLA	C1D-ND	3.76	1.42	1.37
28	BQ	619	XAT	C31-C30	3.76	1.55	1.43
25	y	317	LUT	C10-C9	3.76	1.40	1.35
25	Au	616	LUT	C14-C13	3.76	1.40	1.35
23	y	310	CHL	CHB-C1B	3.76	1.47	1.39
23	BU	607	CHL	CHD-C4C	3.76	1.47	1.39
25	0	616	LUT	C34-C33	3.76	1.40	1.35
23	BJ	605	CHL	OBD-CAD	3.76	1.29	1.22
23	AA	309	CHL	OBD-CAD	3.76	1.29	1.22
29	f	101	BCR	C1-C6	-3.76	1.48	1.53
28	BJ	619	XAT	C35-C34	3.76	1.55	1.43
24	s	611	CLA	C1D-ND	3.76	1.42	1.37
23	BQ	605	CHL	CHD-C4C	3.76	1.47	1.39
28	y	301	XAT	C11-C10	3.75	1.55	1.43
25	7	316	LUT	C30-C29	3.75	1.40	1.35
25	n	616	LUT	C14-C13	3.75	1.40	1.35
24	AB	308	CLA	C4D-ND	-3.75	1.32	1.37
28	7	318	XAT	C35-C34	3.75	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	609	CLA	C1D-ND	3.75	1.42	1.37
25	N	616	LUT	C10-C9	3.75	1.40	1.35
26	5	617	NEX	C30-C29	3.75	1.40	1.35
28	BB	301	XAT	C35-C34	3.75	1.55	1.43
29	Ay	102	BCR	C1-C6	-3.75	1.48	1.53
28	BJ	619	XAT	C15-C14	3.75	1.55	1.43
23	A2	608	CHL	CHD-C4C	3.75	1.47	1.39
25	G	615	LUT	C14-C13	3.75	1.40	1.35
29	v	617	BCR	C1-C6	-3.74	1.48	1.53
23	N	609	CHL	CHD-C4C	3.74	1.47	1.39
23	g	606	CHL	OBD-CAD	3.74	1.28	1.22
23	BJ	607	CHL	OBD-CAD	3.74	1.28	1.22
25	Y	317	LUT	C30-C29	3.74	1.40	1.35
29	v	618	BCR	C1-C6	-3.74	1.48	1.53
25	g	615	LUT	C34-C33	3.74	1.40	1.35
24	s	608	CLA	C1D-ND	3.74	1.42	1.37
25	A2	616	LUT	C34-C33	3.74	1.40	1.35
23	Ba	307	CHL	CHD-C4C	3.74	1.47	1.39
23	n	609	CHL	CHC-C4B	3.74	1.47	1.39
23	n	601	CHL	OBD-CAD	3.73	1.28	1.22
25	N	615	LUT	C14-C13	3.73	1.40	1.35
29	B	617	BCR	C1-C6	-3.73	1.48	1.53
28	5	619	XAT	C11-C10	3.73	1.55	1.43
23	9	609	CHL	CHD-C4C	3.73	1.47	1.39
25	y	316	LUT	C10-C9	3.73	1.40	1.35
28	Ba	301	XAT	C11-C10	3.73	1.55	1.43
23	A6	605	CHL	CHD-C4C	3.73	1.47	1.39
23	9	609	CHL	C4B-NB	-3.73	1.33	1.37
24	g	602	CLA	C1D-ND	3.73	1.42	1.37
23	r	607	CHL	CHD-C4C	3.73	1.47	1.39
23	g	605	CHL	OBD-CAD	3.73	1.28	1.22
29	c	515	BCR	C1-C6	-3.73	1.48	1.53
23	0	605	CHL	OBD-CAD	3.73	1.28	1.22
29	BE	601	BCR	C1-C6	-3.73	1.48	1.53
23	s	607	CHL	OBD-CAD	3.73	1.28	1.22
23	A2	605	CHL	CHD-C4C	3.73	1.47	1.39
24	C	511	CLA	C1D-ND	3.73	1.42	1.37
28	AB	312	XAT	C35-C34	3.73	1.55	1.43
23	7	309	CHL	OBD-CAD	3.73	1.28	1.22
24	7	315	CLA	C1D-ND	3.72	1.42	1.37
32	l	102	SQD	O47-C45	-3.72	1.37	1.46
28	AA	318	XAT	C31-C30	3.72	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	602	CLA	C1D-ND	3.72	1.42	1.37
28	Ba	301	XAT	C31-C30	3.72	1.55	1.43
23	BU	606	CHL	CHD-C4C	3.72	1.47	1.39
28	BQ	619	XAT	C35-C34	3.72	1.55	1.43
23	AA	306	CHL	CHC-C4B	3.72	1.47	1.39
25	G	616	LUT	C30-C29	3.72	1.40	1.35
25	BB	317	LUT	C30-C29	3.72	1.40	1.35
23	r	606	CHL	CHD-C4C	3.72	1.47	1.39
25	BJ	616	LUT	C10-C9	3.72	1.40	1.35
28	N	619	XAT	C11-C10	3.72	1.55	1.43
28	y	301	XAT	C15-C14	3.72	1.55	1.43
28	y	301	XAT	C31-C30	3.72	1.55	1.43
28	r	616	XAT	C31-C30	3.72	1.55	1.43
24	BQ	602	CLA	C1D-ND	3.72	1.42	1.37
23	N	605	CHL	CHD-C4C	3.72	1.47	1.39
24	b	606	CLA	C1D-ND	3.71	1.42	1.37
28	AA	318	XAT	C35-C34	3.71	1.55	1.43
23	y	309	CHL	CHC-C4B	3.71	1.47	1.39
25	Ba	316	LUT	C30-C29	3.71	1.40	1.35
28	n	619	XAT	C15-C14	3.71	1.54	1.43
23	7	306	CHL	CHC-C4B	3.71	1.47	1.39
28	r	616	XAT	C35-C34	3.71	1.54	1.43
24	B	601	CLA	C1D-ND	3.71	1.42	1.37
23	0	609	CHL	CHD-C4C	3.71	1.47	1.39
23	6	605	CHL	OBD-CAD	3.71	1.28	1.22
25	Au	615	LUT	C14-C13	3.71	1.40	1.35
29	BI	101	BCR	C1-C6	-3.71	1.48	1.53
24	BJ	613	CLA	C1D-ND	3.71	1.42	1.37
24	n	611	CLA	C1D-ND	3.70	1.42	1.37
28	Ba	301	XAT	C15-C14	3.70	1.54	1.43
23	Ba	307	CHL	CHC-C4B	3.70	1.47	1.39
28	AA	318	XAT	C15-C14	3.70	1.54	1.43
25	Y	317	LUT	C14-C13	3.70	1.40	1.35
25	Ba	316	LUT	C10-C9	3.70	1.40	1.35
28	7	318	XAT	C31-C30	3.70	1.54	1.43
23	y	307	CHL	CHD-C4C	3.70	1.47	1.39
24	BJ	603	CLA	C1D-ND	3.70	1.42	1.37
23	G	607	CHL	CHD-C4C	3.70	1.47	1.39
28	7	318	XAT	C15-C14	3.70	1.54	1.43
24	BU	614	CLA	C1D-ND	3.70	1.42	1.37
28	BQ	619	XAT	C15-C14	3.70	1.54	1.43
28	n	619	XAT	C35-C34	3.70	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BQ	611	CLA	C1D-ND	3.70	1.42	1.37
28	Ba	301	XAT	C35-C34	3.70	1.54	1.43
24	BE	606	CLA	C1D-ND	3.70	1.42	1.37
24	BU	602	CLA	C4D-ND	-3.69	1.32	1.37
24	BV	610	CLA	C1D-ND	3.69	1.42	1.37
24	n	612	CLA	C1D-ND	3.69	1.42	1.37
24	BQ	612	CLA	C1D-ND	3.69	1.42	1.37
23	BJ	606	CHL	OBD-CAD	3.69	1.28	1.22
23	n	607	CHL	OBD-CAD	3.69	1.28	1.22
24	n	603	CLA	C1D-ND	3.69	1.42	1.37
28	8	312	XAT	C35-C34	3.69	1.54	1.43
24	BE	603	CLA	C1D-ND	3.69	1.42	1.37
24	5	610	CLA	C4D-ND	-3.69	1.32	1.37
23	A2	609	CHL	CHD-C4C	3.69	1.47	1.39
24	s	602	CLA	C1D-ND	3.69	1.42	1.37
26	N	617	NEX	C14-C13	3.69	1.40	1.35
28	BU	616	XAT	C31-C30	3.69	1.54	1.43
24	BQ	613	CLA	C1D-ND	3.69	1.42	1.37
23	BQ	605	CHL	OBD-CAD	3.69	1.28	1.22
25	G	616	LUT	C14-C13	3.69	1.40	1.35
26	BQ	617	NEX	C10-C9	3.69	1.40	1.35
24	g	603	CLA	C1D-ND	3.69	1.42	1.37
23	5	606	CHL	CHD-C4C	3.69	1.47	1.39
23	N	606	CHL	CHD-C4C	3.69	1.47	1.39
25	Au	616	LUT	C30-C29	3.68	1.40	1.35
28	BU	616	XAT	C35-C34	3.68	1.54	1.43
23	Ba	309	CHL	CHC-C4B	3.68	1.47	1.39
25	y	316	LUT	C34-C33	3.68	1.40	1.35
24	BV	612	CLA	C1D-ND	3.68	1.42	1.37
23	N	606	CHL	CHC-C4B	3.68	1.47	1.39
23	y	307	CHL	CHC-C4B	3.68	1.47	1.39
23	s	605	CHL	CHC-C4B	3.68	1.47	1.39
28	9	619	XAT	C31-C30	3.68	1.54	1.43
24	9	603	CLA	C4D-ND	-3.68	1.32	1.37
23	6	609	CHL	CHD-C4C	3.68	1.47	1.39
28	y	301	XAT	C35-C34	3.68	1.54	1.43
24	v	601	CLA	C1D-ND	3.67	1.42	1.37
38	BD	408	PHO	C1D-C2D	3.67	1.43	1.39
24	BV	608	CLA	C1D-ND	3.67	1.42	1.37
38	R	407	PHO	C1D-C2D	3.67	1.43	1.39
23	9	606	CHL	CHD-C4C	3.67	1.47	1.39
23	AA	308	CHL	CHD-C4C	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	615	LUT	C10-C9	3.67	1.40	1.35
25	A2	616	LUT	C10-C9	3.67	1.40	1.35
23	A2	606	CHL	CHD-C4C	3.67	1.47	1.39
25	BB	317	LUT	C14-C13	3.67	1.40	1.35
28	A2	619	XAT	C11-C10	3.67	1.54	1.43
24	BQ	603	CLA	C1D-ND	3.67	1.42	1.37
28	5	619	XAT	C31-C30	3.67	1.54	1.43
23	A2	606	CHL	CHC-C4B	3.67	1.47	1.39
23	7	307	CHL	OBD-CAD	3.67	1.28	1.22
25	Y	317	LUT	C10-C9	3.67	1.40	1.35
25	y	316	LUT	C30-C29	3.67	1.40	1.35
28	AB	312	XAT	C15-C14	3.67	1.54	1.43
24	y	312	CLA	C1D-ND	3.67	1.42	1.37
23	Au	607	CHL	CHD-C4C	3.67	1.47	1.39
23	n	605	CHL	OBD-CAD	3.67	1.28	1.22
25	y	317	LUT	C30-C29	3.67	1.40	1.35
29	b	618	BCR	C1-C6	-3.67	1.48	1.53
25	0	615	LUT	C30-C29	3.67	1.40	1.35
23	n	606	CHL	OBD-CAD	3.67	1.28	1.22
24	n	604	CLA	C1D-ND	3.67	1.42	1.37
29	z	101	BCR	C30-C25	-3.67	1.48	1.53
24	BV	602	CLA	C1D-ND	3.66	1.42	1.37
28	8	312	XAT	C15-C14	3.66	1.54	1.43
23	s	605	CHL	OBD-CAD	3.66	1.28	1.22
23	BQ	606	CHL	OBD-CAD	3.66	1.28	1.22
24	s	610	CLA	C1D-ND	3.66	1.42	1.37
23	8	306	CHL	CHC-C4B	3.66	1.47	1.39
23	g	601	CHL	OBD-CAD	3.66	1.28	1.22
29	B	618	BCR	C1-C6	-3.66	1.48	1.53
23	6	605	CHL	CHC-C4B	3.66	1.47	1.39
24	s	612	CLA	C1D-ND	3.66	1.42	1.37
29	Bb	101	BCR	C30-C25	-3.65	1.48	1.53
24	S	603	CLA	C1D-ND	3.65	1.42	1.37
29	H	101	BCR	C1-C6	-3.65	1.48	1.53
29	b	620	BCR	C1-C6	-3.65	1.48	1.53
25	AA	317	LUT	C34-C33	3.65	1.40	1.35
26	N	617	NEX	C34-C33	3.65	1.40	1.35
23	7	308	CHL	CHD-C4C	3.65	1.47	1.39
25	BJ	615	LUT	C34-C33	3.65	1.40	1.35
23	BV	606	CHL	OBD-CAD	3.65	1.28	1.22
24	n	614	CLA	C4B-NB	3.64	1.42	1.37
24	y	303	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	615	LUT	C8-C9	-3.64	1.38	1.45
23	BV	605	CHL	CHC-C4B	3.64	1.47	1.39
28	5	619	XAT	C35-C34	3.64	1.54	1.43
26	A2	617	NEX	C34-C33	3.64	1.40	1.35
29	Av	101	BCR	C1-C6	-3.64	1.48	1.53
25	BJ	615	LUT	C30-C29	3.64	1.40	1.35
23	BV	607	CHL	CHC-C4B	3.64	1.47	1.39
29	BE	620	BCR	C1-C6	-3.64	1.48	1.53
28	9	619	XAT	C35-C34	3.64	1.54	1.43
23	0	601	CHL	CHC-C4B	3.64	1.47	1.39
24	b	603	CLA	C1D-ND	3.64	1.42	1.37
24	Ba	303	CLA	C1D-ND	3.63	1.42	1.37
29	K	102	BCR	C30-C25	-3.63	1.48	1.53
23	G	606	CHL	OBD-CAD	3.63	1.28	1.22
25	Ba	317	LUT	C30-C29	3.63	1.40	1.35
23	6	606	CHL	CHD-C4C	3.63	1.47	1.39
23	S	601	CHL	CHC-C4B	3.63	1.47	1.39
24	B	606	CLA	C1D-ND	3.63	1.42	1.37
25	BB	316	LUT	C14-C13	3.63	1.40	1.35
23	6	608	CHL	OBD-CAD	3.63	1.28	1.22
24	9	610	CLA	C4D-ND	-3.63	1.32	1.37
23	N	607	CHL	CHD-C4C	3.63	1.47	1.39
24	BQ	604	CLA	C1D-ND	3.63	1.42	1.37
23	BV	605	CHL	OBD-CAD	3.63	1.28	1.22
29	z	102	BCR	C30-C25	-3.63	1.48	1.53
24	y	304	CLA	C1D-ND	3.63	1.42	1.37
23	0	605	CHL	CHC-C4B	3.63	1.47	1.39
25	y	316	LUT	C14-C13	3.63	1.40	1.35
23	y	309	CHL	CHB-C1B	3.63	1.47	1.39
24	A6	603	CLA	C1D-ND	3.63	1.42	1.37
23	6	607	CHL	OBD-CAD	3.62	1.28	1.22
23	n	606	CHL	CHC-C4B	3.62	1.47	1.39
24	AB	301	CLA	C1D-ND	3.62	1.42	1.37
28	r	616	XAT	C15-C14	3.62	1.54	1.43
23	s	606	CHL	OBD-CAD	3.62	1.28	1.22
23	9	607	CHL	CHD-C4C	3.62	1.47	1.39
24	BU	601	CLA	C4D-ND	-3.62	1.32	1.37
23	BQ	607	CHL	OBD-CAD	3.62	1.28	1.22
23	G	609	CHL	CHB-C1B	3.62	1.47	1.39
24	BJ	602	CLA	C1D-ND	3.62	1.42	1.37
24	Au	614	CLA	C1D-ND	3.61	1.42	1.37
25	Y	316	LUT	C14-C13	3.61	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	617	NEX	C30-C29	3.61	1.40	1.35
23	BJ	601	CHL	OBD-CAD	3.61	1.28	1.22
24	Ba	313	CLA	C1D-ND	3.61	1.42	1.37
23	5	609	CHL	C2C-C3C	3.61	1.44	1.36
23	n	608	CHL	OBD-CAD	3.61	1.28	1.22
23	BQ	608	CHL	OBD-CAD	3.61	1.28	1.22
24	AB	302	CLA	C4D-ND	-3.61	1.32	1.37
24	8	309	CLA	C1D-ND	3.61	1.42	1.37
23	5	605	CHL	OBD-CAD	3.61	1.28	1.22
23	7	308	CHL	OBD-CAD	3.61	1.28	1.22
23	G	607	CHL	OBD-CAD	3.60	1.28	1.22
23	A2	607	CHL	CHD-C4C	3.60	1.47	1.39
23	Au	607	CHL	OBD-CAD	3.60	1.28	1.22
26	A2	617	NEX	C19-C9	-3.60	1.43	1.50
23	6	601	CHL	CHC-C4B	3.60	1.47	1.39
23	e	601	CHL	OBD-CAD	3.60	1.28	1.22
23	AB	306	CHL	CHC-C4B	3.60	1.47	1.39
24	r	602	CLA	C4D-ND	-3.60	1.32	1.37
25	A2	615	LUT	C14-C13	3.60	1.40	1.35
24	G	614	CLA	C1D-ND	3.60	1.42	1.37
24	8	310	CLA	C1D-ND	3.60	1.42	1.37
24	y	314	CLA	C1D-ND	3.60	1.42	1.37
23	y	306	CHL	OBD-CAD	3.60	1.28	1.22
23	BQ	607	CHL	CHC-C4B	3.60	1.47	1.39
23	0	608	CHL	OBD-CAD	3.60	1.28	1.22
23	A6	601	CHL	CHC-C4B	3.60	1.47	1.39
23	y	307	CHL	OBD-CAD	3.59	1.28	1.22
23	AA	307	CHL	OBD-CAD	3.59	1.28	1.22
24	AB	309	CLA	C1D-ND	3.59	1.42	1.37
24	BQ	614	CLA	C4B-NB	3.59	1.42	1.37
28	5	619	XAT	C15-C14	3.59	1.54	1.43
23	BQ	606	CHL	CHC-C4B	3.59	1.47	1.39
28	BU	616	XAT	C15-C14	3.59	1.54	1.43
23	s	607	CHL	CHC-C4B	3.59	1.47	1.39
23	AA	308	CHL	OBD-CAD	3.59	1.28	1.22
26	Y	318	NEX	C30-C29	3.59	1.40	1.35
24	5	603	CLA	C4D-ND	-3.59	1.32	1.37
24	v	606	CLA	C1D-ND	3.59	1.42	1.37
23	Au	606	CHL	OBD-CAD	3.59	1.28	1.22
23	BH	601	CHL	OBD-CAD	3.59	1.28	1.22
32	2	408	SQD	O47-C45	-3.59	1.37	1.46
24	b	602	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Ba	312	CLA	C1D-ND	3.59	1.42	1.37
24	B	616	CLA	C1D-ND	3.58	1.42	1.37
24	Ba	314	CLA	C1D-ND	3.58	1.42	1.37
25	BB	317	LUT	C10-C9	3.58	1.40	1.35
23	n	607	CHL	CHC-C4B	3.58	1.47	1.39
24	Au	604	CLA	C1D-ND	3.58	1.42	1.37
24	b	616	CLA	C1D-ND	3.58	1.42	1.37
23	G	605	CHL	CHC-C4B	3.58	1.47	1.39
29	v	619	BCR	C1-C6	-3.58	1.48	1.53
24	b	617	CLA	C1D-ND	3.58	1.42	1.37
24	BE	602	CLA	C1D-ND	3.58	1.42	1.37
24	BE	616	CLA	C1D-ND	3.58	1.42	1.37
23	Y	308	CHL	CHD-C4C	3.58	1.47	1.39
23	8	305	CHL	OBD-CAD	3.58	1.28	1.22
38	a	409	PHO	C4D-CHA	3.58	1.45	1.39
24	B	602	CLA	C1D-ND	3.57	1.42	1.37
24	5	612	CLA	C1D-ND	3.57	1.42	1.37
23	n	609	CHL	OBD-CAD	3.57	1.28	1.22
23	9	605	CHL	OBD-CAD	3.57	1.28	1.22
29	b	601	BCR	C1-C6	-3.57	1.48	1.53
26	BB	320	NEX	C30-C29	3.57	1.40	1.35
24	BU	609	CLA	C4D-ND	-3.57	1.32	1.37
23	5	609	CHL	CHB-C1B	3.57	1.47	1.39
29	Ay	102	BCR	C30-C25	-3.57	1.48	1.53
29	B	619	BCR	C1-C6	-3.57	1.48	1.53
24	y	311	CLA	C1D-ND	3.57	1.42	1.37
24	8	301	CLA	C1D-ND	3.57	1.42	1.37
26	Ba	318	NEX	C10-C9	3.56	1.40	1.35
24	BE	617	CLA	C1D-ND	3.56	1.42	1.37
25	7	317	LUT	C30-C29	3.56	1.40	1.35
32	BG	406	SQD	O47-C45	-3.56	1.37	1.46
23	S	607	CHL	CHD-C4C	3.56	1.47	1.39
29	R	410	BCR	C30-C25	-3.56	1.48	1.53
24	r	609	CLA	C4D-ND	-3.56	1.32	1.37
29	A	411	BCR	C30-C25	-3.56	1.48	1.53
23	Ba	307	CHL	OBD-CAD	3.56	1.28	1.22
24	G	604	CLA	C1D-ND	3.56	1.42	1.37
23	Ba	308	CHL	OBD-CAD	3.56	1.28	1.22
24	8	302	CLA	C4D-ND	-3.56	1.32	1.37
23	S	605	CHL	OBD-CAD	3.56	1.28	1.22
24	g	612	CLA	C4B-NB	3.55	1.42	1.37
24	v	616	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BJ	612	CLA	C4B-NB	3.55	1.42	1.37
24	BU	611	CLA	C4D-ND	-3.55	1.32	1.37
26	r	617	NEX	C30-C29	3.55	1.40	1.35
24	G	611	CLA	C4D-ND	-3.55	1.32	1.37
23	s	601	CHL	OBD-CAD	3.55	1.28	1.22
23	0	606	CHL	CHD-C4C	3.55	1.47	1.39
32	R	411	SQD	O47-C45	-3.55	1.37	1.46
23	AA	306	CHL	CHB-C1B	3.55	1.47	1.39
24	Ba	304	CLA	C1D-ND	3.55	1.42	1.37
23	y	308	CHL	OBD-CAD	3.55	1.28	1.22
24	b	608	CLA	C1D-ND	3.55	1.42	1.37
24	7	304	CLA	C4D-ND	-3.55	1.32	1.37
25	g	615	LUT	C30-C29	3.55	1.40	1.35
23	0	609	CHL	C4B-NB	-3.55	1.33	1.37
23	A6	605	CHL	CHC-C4B	3.55	1.47	1.39
24	Ba	311	CLA	C1D-ND	3.55	1.42	1.37
23	A6	605	CHL	OBD-CAD	3.55	1.28	1.22
24	y	313	CLA	C1D-ND	3.54	1.42	1.37
32	d	406	SQD	O47-C45	-3.54	1.37	1.46
23	Ba	306	CHL	OBD-CAD	3.54	1.28	1.22
24	S	610	CLA	C1D-ND	3.54	1.42	1.37
24	BE	608	CLA	C1D-ND	3.54	1.42	1.37
24	S	612	CLA	C1D-ND	3.54	1.42	1.37
24	A6	610	CLA	C1D-ND	3.54	1.42	1.37
23	y	307	CHL	CHB-C1B	3.54	1.47	1.39
24	6	603	CLA	C4D-ND	-3.54	1.32	1.37
38	BD	409	PHO	C4D-CHA	3.54	1.45	1.39
24	N	614	CLA	C4B-NB	3.54	1.42	1.37
23	7	306	CHL	CHB-C1B	3.54	1.47	1.39
24	Y	311	CLA	C4D-ND	-3.54	1.32	1.37
32	BD	412	SQD	O47-C45	-3.54	1.37	1.46
24	Au	613	CLA	C1D-ND	3.54	1.42	1.37
25	8	311	LUT	C30-C29	3.54	1.40	1.35
23	BQ	609	CHL	OBD-CAD	3.53	1.28	1.22
23	6	606	CHL	OBD-CAD	3.53	1.28	1.22
23	0	607	CHL	OBD-CAD	3.53	1.28	1.22
23	G	609	CHL	CHC-C4B	3.53	1.47	1.39
23	9	609	CHL	CHB-C1B	3.53	1.47	1.39
23	S	601	CHL	OBD-CAD	3.53	1.28	1.22
23	AB	305	CHL	OBD-CAD	3.53	1.28	1.22
24	n	610	CLA	C1D-ND	3.53	1.42	1.37
24	7	312	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	410	CLA	C1D-ND	3.53	1.42	1.37
23	AB	307	CHL	CHC-C4B	3.53	1.47	1.39
31	d	403	PL9	C26-C27	3.53	1.65	1.53
24	A2	614	CLA	C4B-NB	3.53	1.42	1.37
24	BQ	610	CLA	C1D-ND	3.53	1.42	1.37
23	9	601	CHL	OBD-CAD	3.53	1.28	1.22
23	S	607	CHL	C2C-C3C	3.53	1.44	1.36
23	Ba	309	CHL	CHB-C1B	3.53	1.47	1.39
24	r	611	CLA	C4D-ND	-3.53	1.32	1.37
23	n	608	CHL	CHC-C4B	3.53	1.47	1.39
23	g	606	CHL	CHC-C4B	3.53	1.47	1.39
24	b	605	CLA	C1D-ND	3.52	1.42	1.37
24	v	603	CLA	C1D-ND	3.52	1.42	1.37
23	s	607	CHL	CHB-C1B	3.52	1.47	1.39
23	y	302	CHL	CHC-C4B	3.52	1.47	1.39
23	BV	601	CHL	OBD-CAD	3.52	1.28	1.22
24	Au	612	CLA	C1D-ND	3.52	1.42	1.37
23	BJ	607	CHL	CHC-C4B	3.52	1.47	1.39
25	7	317	LUT	C14-C13	3.52	1.40	1.35
25	BB	316	LUT	C10-C9	3.52	1.40	1.35
23	A6	607	CHL	OBD-CAD	3.52	1.28	1.22
25	N	616	LUT	C30-C29	3.52	1.40	1.35
25	BU	615	LUT	C14-C13	3.52	1.40	1.35
23	BJ	606	CHL	CHC-C4B	3.52	1.47	1.39
24	b	609	CLA	C1D-ND	3.52	1.42	1.37
24	BF	508	CLA	C4D-ND	-3.52	1.32	1.37
23	r	613	CHL	OBD-CAD	3.52	1.28	1.22
23	BB	308	CHL	CHD-C4C	3.52	1.47	1.39
24	AA	304	CLA	C4D-ND	-3.52	1.32	1.37
32	A	413	SQD	O47-C45	-3.52	1.37	1.46
24	BB	303	CLA	C4D-ND	-3.52	1.32	1.37
29	a	411	BCR	C30-C25	-3.52	1.48	1.53
23	n	608	CHL	CHB-C1B	3.52	1.47	1.39
24	0	603	CLA	C4D-ND	-3.51	1.32	1.37
24	v	612	CLA	C4D-ND	-3.51	1.32	1.37
24	2	402	CLA	C4D-ND	-3.51	1.32	1.37
23	BQ	606	CHL	CHB-C1B	3.51	1.47	1.39
23	S	607	CHL	OBD-CAD	3.51	1.28	1.22
23	A6	606	CHL	OBD-CAD	3.51	1.28	1.22
23	S	605	CHL	CHC-C4B	3.51	1.47	1.39
32	L	103	SQD	O47-C45	-3.51	1.37	1.46
25	AB	311	LUT	C10-C9	3.51	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	601	CLA	C4D-ND	-3.51	1.32	1.37
23	5	601	CHL	OBD-CAD	3.51	1.28	1.22
24	s	613	CLA	C1D-ND	3.51	1.42	1.37
23	8	304	CHL	CHC-C4B	3.51	1.47	1.39
23	G	601	CHL	OBD-CAD	3.51	1.28	1.22
24	S	611	CLA	C1D-ND	3.50	1.42	1.37
23	y	302	CHL	OBD-CAD	3.50	1.28	1.22
29	BD	411	BCR	C30-C25	-3.50	1.49	1.53
23	Ba	302	CHL	OBD-CAD	3.50	1.28	1.22
38	A	409	PHO	C4D-CHA	3.50	1.45	1.39
23	5	601	CHL	CHC-C4B	3.50	1.47	1.39
23	9	601	CHL	CHC-C4B	3.50	1.47	1.39
23	BQ	608	CHL	CHC-C4B	3.50	1.47	1.39
24	b	604	CLA	C1D-ND	3.50	1.42	1.37
24	Ba	305	CLA	C1D-ND	3.50	1.42	1.37
23	Ba	307	CHL	CHB-C1B	3.50	1.47	1.39
24	B	607	CLA	C1D-ND	3.50	1.42	1.37
23	0	606	CHL	OBD-CAD	3.50	1.28	1.22
23	n	601	CHL	CHC-C4B	3.50	1.47	1.39
24	AA	312	CLA	C1D-ND	3.50	1.42	1.37
25	r	615	LUT	C14-C13	3.49	1.40	1.35
23	Y	307	CHL	OBD-CAD	3.49	1.28	1.22
24	AB	310	CLA	C1D-ND	3.49	1.42	1.37
23	Ba	302	CHL	CHC-C4B	3.49	1.47	1.39
23	BQ	608	CHL	CHB-C1B	3.49	1.47	1.39
23	S	606	CHL	OBD-CAD	3.49	1.28	1.22
24	A6	608	CLA	C1D-ND	3.49	1.42	1.37
23	5	607	CHL	OBD-CAD	3.49	1.28	1.22
23	AB	304	CHL	CHC-C4B	3.49	1.47	1.39
23	8	306	CHL	OBD-CAD	3.49	1.28	1.22
29	B	617	BCR	C30-C25	-3.49	1.49	1.53
26	7	319	NEX	C10-C9	3.49	1.40	1.35
25	Y	316	LUT	C10-C9	3.49	1.40	1.35
32	a	412	SQD	O47-C45	-3.49	1.37	1.46
23	AB	306	CHL	OBD-CAD	3.49	1.28	1.22
24	BB	311	CLA	C4D-ND	-3.49	1.32	1.37
32	A1	101	SQD	O5-C1	3.49	1.50	1.41
32	L	103	SQD	O5-C1	3.48	1.50	1.41
32	A1	101	SQD	O47-C45	-3.48	1.37	1.46
24	G	612	CLA	C1D-ND	3.48	1.42	1.37
23	BV	607	CHL	CHB-C1B	3.48	1.47	1.39
24	b	612	CLA	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	607	CHL	CHC-C4B	3.48	1.47	1.39
24	B	605	CLA	C1D-ND	3.48	1.42	1.37
24	y	305	CLA	C1D-ND	3.48	1.42	1.37
24	v	605	CLA	C1D-ND	3.48	1.42	1.37
24	N	610	CLA	C4D-ND	-3.48	1.32	1.37
23	G	608	CHL	OBD-CAD	3.48	1.28	1.22
24	BE	605	CLA	C1D-ND	3.48	1.42	1.37
23	s	606	CHL	CHC-C4B	3.48	1.47	1.39
23	y	306	CHL	CHC-C4B	3.48	1.47	1.39
23	9	607	CHL	OBD-CAD	3.48	1.28	1.22
23	Ba	306	CHL	CHC-C4B	3.48	1.47	1.39
25	S	615	LUT	C10-C9	3.48	1.40	1.35
23	0	608	CHL	CHC-C4B	3.48	1.47	1.39
24	N	613	CLA	C1D-ND	3.48	1.42	1.37
23	BQ	601	CHL	CHC-C4B	3.48	1.47	1.39
24	a	407	CLA	C1D-ND	3.48	1.42	1.37
24	BD	407	CLA	C1D-ND	3.48	1.42	1.37
24	7	305	CLA	C1D-ND	3.48	1.42	1.37
26	BB	318	NEX	C30-C29	3.47	1.40	1.35
29	v	617	BCR	C30-C25	-3.47	1.49	1.53
24	c	508	CLA	C4D-ND	-3.47	1.32	1.37
23	5	605	CHL	CHC-C4B	3.47	1.47	1.39
23	8	304	CHL	CHB-C1B	3.47	1.47	1.39
23	n	606	CHL	CHB-C1B	3.47	1.47	1.39
29	BK	101	BCR	C1-C6	-3.47	1.49	1.53
24	y	315	CLA	C1D-ND	3.47	1.42	1.37
25	AA	317	LUT	C30-C29	3.47	1.40	1.35
24	G	613	CLA	C1D-ND	3.47	1.42	1.37
24	9	612	CLA	C1D-ND	3.47	1.42	1.37
24	Ba	304	CLA	C4B-NB	3.47	1.42	1.37
24	0	613	CLA	C4D-ND	-3.47	1.32	1.37
24	S	608	CLA	C1D-ND	3.47	1.42	1.37
24	b	607	CLA	C1D-ND	3.46	1.42	1.37
25	AA	317	LUT	C14-C13	3.46	1.40	1.35
24	A2	613	CLA	C1D-ND	3.46	1.42	1.37
23	BU	613	CHL	OBD-CAD	3.46	1.28	1.22
23	AA	310	CHL	CHC-C4B	3.46	1.47	1.39
24	v	602	CLA	C1D-ND	3.46	1.42	1.37
24	BU	612	CLA	C4D-ND	-3.46	1.32	1.37
24	BF	510	CLA	C4D-ND	-3.46	1.32	1.37
23	AB	304	CHL	CHB-C1B	3.46	1.47	1.39
23	BJ	605	CHL	CHC-C4B	3.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AA	319	NEX	C10-C9	3.46	1.40	1.35
24	0	614	CLA	C4D-ND	-3.46	1.32	1.37
24	BF	513	CLA	C4D-ND	-3.46	1.32	1.37
24	S	602	CLA	C1D-ND	3.46	1.42	1.37
23	BB	308	CHL	OBD-CAD	3.46	1.28	1.22
23	7	310	CHL	OBD-CAD	3.45	1.28	1.22
23	BU	607	CHL	OBD-CAD	3.45	1.28	1.22
24	r	610	CLA	C4D-ND	-3.45	1.32	1.37
24	A6	611	CLA	C1D-ND	3.45	1.42	1.37
24	A2	610	CLA	C4D-ND	-3.45	1.32	1.37
23	9	605	CHL	CHC-C4B	3.45	1.47	1.39
23	6	608	CHL	CHC-C4B	3.45	1.47	1.39
25	AA	316	LUT	C10-C9	3.45	1.40	1.35
24	D	401	CLA	C4D-ND	-3.45	1.33	1.37
24	AB	303	CLA	C4D-ND	-3.45	1.33	1.37
24	BF	505	CLA	C1D-ND	3.45	1.42	1.37
23	BU	605	CHL	OBD-CAD	3.45	1.28	1.22
26	g	617	NEX	C10-C9	3.45	1.40	1.35
23	BV	606	CHL	CHC-C4B	3.45	1.47	1.39
24	B	603	CLA	C1D-ND	3.45	1.42	1.37
24	B	612	CLA	C4D-ND	-3.45	1.33	1.37
23	Au	605	CHL	CHC-C4B	3.45	1.47	1.39
23	Au	606	CHL	CHC-C4B	3.45	1.47	1.39
23	6	601	CHL	OBD-CAD	3.45	1.28	1.22
23	8	307	CHL	OBD-CAD	3.45	1.28	1.22
26	N	617	NEX	C30-C29	3.45	1.40	1.35
24	1	507	CLA	C4D-ND	-3.45	1.33	1.37
24	BE	604	CLA	C1D-ND	3.44	1.42	1.37
23	Y	302	CHL	OBD-CAD	3.44	1.28	1.22
23	Y	306	CHL	CHC-C4B	3.44	1.47	1.39
24	BE	612	CLA	C1D-ND	3.44	1.42	1.37
24	6	612	CLA	C4D-ND	-3.44	1.33	1.37
24	C	507	CLA	C4D-ND	-3.44	1.33	1.37
24	BD	406	CLA	C4D-ND	-3.44	1.33	1.37
23	g	609	CHL	OBD-CAD	3.44	1.28	1.22
23	N	609	CHL	CHC-C4B	3.44	1.47	1.39
24	BD	410	CLA	C1D-ND	3.44	1.42	1.37
24	6	613	CLA	C4D-ND	-3.44	1.33	1.37
23	G	606	CHL	CHC-C4B	3.44	1.47	1.39
23	g	605	CHL	CHC-C4B	3.44	1.47	1.39
24	BF	512	CLA	C1D-ND	3.44	1.42	1.37
25	A2	616	LUT	C30-C29	3.44	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C1D-ND	3.44	1.42	1.37
25	AB	311	LUT	C34-C33	3.44	1.40	1.35
23	AA	310	CHL	OBD-CAD	3.44	1.28	1.22
23	Au	601	CHL	OBD-CAD	3.44	1.28	1.22
25	6	615	LUT	C30-C29	3.44	1.40	1.35
23	g	609	CHL	CHB-C1B	3.44	1.47	1.39
24	5	613	CLA	C1D-ND	3.44	1.42	1.37
32	a	412	SQD	O5-C1	3.44	1.50	1.41
23	5	608	CHL	OBD-CAD	3.44	1.28	1.22
32	l	101	SQD	O5-C1	3.44	1.50	1.41
32	BD	412	SQD	O5-C1	3.44	1.50	1.41
24	0	611	CLA	C4D-ND	-3.43	1.33	1.37
23	8	304	CHL	OBD-CAD	3.43	1.28	1.22
24	5	611	CLA	C1D-ND	3.43	1.42	1.37
23	0	601	CHL	OBD-CAD	3.43	1.28	1.22
26	Y	318	NEX	C10-C9	3.43	1.40	1.35
23	e	601	CHL	CHC-C4B	3.43	1.47	1.39
24	y	304	CLA	C4B-NB	3.43	1.42	1.37
24	R	409	CLA	C1D-ND	3.43	1.42	1.37
23	Y	309	CHL	CHC-C4B	3.43	1.47	1.39
24	Ba	315	CLA	C1D-ND	3.43	1.42	1.37
23	6	605	CHL	CHB-C1B	3.43	1.47	1.39
31	D	403	PL9	C52-C5	-3.43	1.43	1.50
24	B	610	CLA	C1D-ND	3.43	1.42	1.37
24	9	604	CLA	C4D-ND	-3.43	1.33	1.37
26	r	617	NEX	C10-C9	3.43	1.40	1.35
24	BU	610	CLA	C4D-ND	-3.43	1.33	1.37
24	b	607	CLA	C4B-NB	3.43	1.42	1.37
24	1	511	CLA	C1D-ND	3.43	1.42	1.37
23	Au	608	CHL	OBD-CAD	3.42	1.28	1.22
23	r	607	CHL	OBD-CAD	3.42	1.28	1.22
24	0	612	CLA	C4D-ND	-3.42	1.33	1.37
23	BB	307	CHL	OBD-CAD	3.42	1.28	1.22
23	r	605	CHL	OBD-CAD	3.42	1.28	1.22
24	b	615	CLA	C1D-ND	3.42	1.42	1.37
24	BV	613	CLA	C1D-ND	3.42	1.42	1.37
24	BF	511	CLA	C4D-ND	-3.42	1.33	1.37
32	BO	101	SQD	O5-C1	3.42	1.50	1.41
24	8	303	CLA	C4D-ND	-3.42	1.33	1.37
24	c	503	CLA	C4D-ND	-3.42	1.33	1.37
24	BE	607	CLA	C4B-NB	3.42	1.42	1.37
23	A6	601	CHL	OBD-CAD	3.42	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	614	CLA	C4D-ND	-3.42	1.33	1.37
23	n	605	CHL	CHC-C4B	3.42	1.47	1.39
24	BE	607	CLA	C1D-ND	3.42	1.42	1.37
23	Au	609	CHL	OBD-CAD	3.42	1.28	1.22
23	A2	608	CHL	CHB-C1B	3.42	1.47	1.39
38	R	408	PHO	C4D-CHA	3.42	1.45	1.39
24	BF	503	CLA	C4D-ND	-3.42	1.33	1.37
23	G	607	CHL	CHC-C4B	3.42	1.47	1.39
24	A	405	CLA	C1D-ND	3.41	1.42	1.37
24	B	604	CLA	C1D-ND	3.41	1.42	1.37
24	A	410	CLA	C1D-ND	3.41	1.42	1.37
29	B	618	BCR	C30-C25	-3.41	1.49	1.53
23	A2	607	CHL	OBD-CAD	3.41	1.28	1.22
24	D	402	CLA	C1D-ND	3.41	1.42	1.37
24	c	513	CLA	C4D-ND	-3.41	1.33	1.37
24	BF	504	CLA	C4D-ND	-3.41	1.33	1.37
23	BH	601	CHL	CHC-C4B	3.41	1.47	1.39
24	B	614	CLA	C1D-ND	3.41	1.42	1.37
24	6	602	CLA	C4D-ND	-3.41	1.33	1.37
24	A6	602	CLA	C1D-ND	3.41	1.42	1.37
23	6	609	CHL	C4B-NB	-3.41	1.33	1.37
23	BJ	609	CHL	CHB-C1B	3.41	1.47	1.39
24	7	311	CLA	C1D-ND	3.41	1.42	1.37
24	AA	303	CLA	C4D-ND	-3.41	1.33	1.37
24	BB	312	CLA	C4D-ND	-3.41	1.33	1.37
24	BG	401	CLA	C4D-ND	-3.41	1.33	1.37
23	7	302	CHL	OBD-CAD	3.41	1.28	1.22
23	N	607	CHL	OBD-CAD	3.41	1.28	1.22
23	g	601	CHL	CHC-C4B	3.40	1.47	1.39
24	6	612	CLA	C1D-ND	3.40	1.42	1.37
23	A2	601	CHL	OBD-CAD	3.40	1.28	1.22
23	A2	609	CHL	CHC-C4B	3.40	1.47	1.39
23	Y	307	CHL	CHD-C4C	3.40	1.47	1.39
24	A	407	CLA	C1D-ND	3.40	1.42	1.37
24	C	505	CLA	C1D-ND	3.40	1.42	1.37
32	D	406	SQD	O47-C45	-3.40	1.38	1.46
24	v	607	CLA	C1D-ND	3.40	1.42	1.37
24	8	308	CLA	C4D-ND	-3.40	1.33	1.37
24	BG	402	CLA	C1D-ND	3.40	1.42	1.37
24	Au	611	CLA	C1D-ND	3.40	1.42	1.37
23	Ba	308	CHL	CHC-C4B	3.40	1.47	1.39
24	6	604	CLA	C4D-ND	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	316	LUT	C10-C9	3.40	1.40	1.35
25	A6	615	LUT	C10-C9	3.40	1.40	1.35
23	7	310	CHL	CHC-C4B	3.40	1.47	1.39
24	AA	305	CLA	C1D-ND	3.40	1.42	1.37
24	Y	303	CLA	C4D-ND	-3.39	1.33	1.37
23	N	601	CHL	OBD-CAD	3.39	1.28	1.22
24	v	606	CLA	C4B-NB	3.39	1.42	1.37
24	0	612	CLA	C1D-ND	3.39	1.42	1.37
24	BQ	611	CLA	C4B-NB	3.39	1.42	1.37
23	N	606	CHL	OBD-CAD	3.39	1.28	1.22
23	AB	307	CHL	OBD-CAD	3.39	1.28	1.22
24	R	406	CLA	C1D-ND	3.39	1.42	1.37
23	N	608	CHL	OBD-CAD	3.39	1.28	1.22
24	r	612	CLA	C4D-ND	-3.39	1.33	1.37
24	1	509	CLA	C4D-ND	-3.39	1.33	1.37
23	BJ	609	CHL	OBD-CAD	3.39	1.28	1.22
24	C	509	CLA	C4D-ND	-3.39	1.33	1.37
24	BV	604	CLA	C3B-C4B	3.39	1.50	1.42
24	BB	305	CLA	C1D-ND	3.39	1.41	1.37
23	BB	306	CHL	CHC-C4B	3.39	1.47	1.39
24	Y	305	CLA	C1D-ND	3.39	1.41	1.37
23	G	605	CHL	CHB-C1B	3.39	1.47	1.39
23	BQ	605	CHL	CHC-C4B	3.39	1.47	1.39
24	BU	608	CLA	C4D-ND	-3.39	1.33	1.37
23	0	605	CHL	CHB-C1B	3.39	1.47	1.39
24	g	604	CLA	C4B-NB	3.38	1.41	1.37
24	d	402	CLA	C1D-ND	3.38	1.41	1.37
23	AB	304	CHL	OBD-CAD	3.38	1.28	1.22
23	Y	306	CHL	CHB-C1B	3.38	1.47	1.39
23	BJ	601	CHL	CHC-C4B	3.38	1.47	1.39
23	5	607	CHL	CHC-C4B	3.38	1.47	1.39
23	BB	309	CHL	CHC-C4B	3.38	1.47	1.39
23	8	307	CHL	CHC-C4B	3.38	1.47	1.39
26	A2	617	NEX	C30-C29	3.38	1.40	1.35
24	c	510	CLA	C4D-ND	-3.38	1.33	1.37
23	Y	309	CHL	OBD-CAD	3.38	1.28	1.22
23	N	608	CHL	CHC-C4B	3.38	1.47	1.39
24	c	512	CLA	C1D-ND	3.38	1.41	1.37
23	Y	308	CHL	OBD-CAD	3.38	1.28	1.22
31	d	403	PL9	C6-C1	-3.38	1.42	1.48
23	N	608	CHL	CHB-C1B	3.38	1.47	1.39
23	0	609	CHL	CHB-C1B	3.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	h	101	BCR	C1-C6	-3.38	1.49	1.53
24	AA	305	CLA	C4D-ND	-3.38	1.33	1.37
24	1	503	CLA	C4D-ND	-3.38	1.33	1.37
24	BF	507	CLA	C4D-ND	-3.38	1.33	1.37
23	A2	606	CHL	OBD-CAD	3.37	1.28	1.22
24	r	608	CLA	C4D-ND	-3.37	1.33	1.37
23	AB	305	CHL	CHC-C4B	3.37	1.47	1.39
24	B	615	CLA	C1D-ND	3.37	1.41	1.37
24	N	611	CLA	C1D-ND	3.37	1.41	1.37
24	c	509	CLA	C1D-ND	3.37	1.41	1.37
24	BE	613	CLA	C4D-ND	-3.37	1.33	1.37
23	BQ	601	CHL	CHB-C1B	3.37	1.47	1.39
24	A6	612	CLA	C1D-ND	3.37	1.41	1.37
24	9	613	CLA	C1D-ND	3.37	1.41	1.37
23	5	606	CHL	OBD-CAD	3.37	1.28	1.22
25	8	311	LUT	C14-C13	3.37	1.40	1.35
23	A6	606	CHL	CHC-C4B	3.37	1.47	1.39
23	5	608	CHL	CHC-C4B	3.37	1.47	1.39
23	8	305	CHL	CHC-C4B	3.37	1.47	1.39
29	Ay	101	BCR	C1-C6	-3.37	1.49	1.53
23	Y	306	CHL	OBD-CAD	3.37	1.28	1.22
23	A2	608	CHL	CHC-C4B	3.37	1.47	1.39
24	0	604	CLA	C1D-ND	3.37	1.41	1.37
24	B	611	CLA	C1D-ND	3.37	1.41	1.37
24	9	611	CLA	C1D-ND	3.37	1.41	1.37
32	BG	406	SQD	O5-C1	3.36	1.50	1.41
24	Y	312	CLA	C4D-ND	-3.36	1.33	1.37
23	9	608	CHL	OBD-CAD	3.36	1.28	1.22
24	9	602	CLA	C1D-ND	3.36	1.41	1.37
23	BU	613	CHL	CHC-C4B	3.36	1.47	1.39
24	G	602	CLA	C4D-ND	-3.36	1.33	1.37
29	b	619	BCR	C1-C6	-3.36	1.49	1.53
24	7	303	CLA	C4D-ND	-3.36	1.33	1.37
24	0	602	CLA	C4D-ND	-3.36	1.33	1.37
26	y	318	NEX	C10-C9	3.36	1.40	1.35
24	5	602	CLA	C1D-ND	3.36	1.41	1.37
24	A6	604	CLA	C1D-ND	3.36	1.41	1.37
24	BB	314	CLA	C4D-ND	-3.36	1.33	1.37
38	A	409	PHO	C1D-C2D	3.36	1.43	1.39
32	R	411	SQD	O5-C1	3.36	1.50	1.41
31	d	403	PL9	C30-C29	-3.36	1.42	1.50
24	5	604	CLA	C4D-ND	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	404	CLA	C1D-ND	3.36	1.41	1.37
23	r	613	CHL	CHC-C4B	3.36	1.46	1.39
32	d	406	SQD	O5-C1	3.36	1.50	1.41
24	7	313	CLA	C1D-ND	3.36	1.41	1.37
23	Y	309	CHL	CHB-C1B	3.36	1.46	1.39
24	A	406	CLA	C4D-ND	-3.36	1.33	1.37
23	y	308	CHL	CHC-C4B	3.36	1.46	1.39
32	BO	101	SQD	O47-C45	-3.36	1.38	1.46
23	S	607	CHL	CHB-C1B	3.36	1.46	1.39
24	0	613	CLA	C1D-ND	3.36	1.41	1.37
24	BF	502	CLA	C1D-ND	3.36	1.41	1.37
24	c	504	CLA	C1D-ND	3.36	1.41	1.37
24	G	603	CLA	C1D-ND	3.35	1.41	1.37
32	BO	101	SQD	O47-C7	3.35	1.43	1.34
24	v	611	CLA	C1D-ND	3.35	1.41	1.37
23	S	606	CHL	CHC-C4B	3.35	1.46	1.39
23	BB	302	CHL	CHC-C4B	3.35	1.46	1.39
24	B	613	CLA	C1D-ND	3.35	1.41	1.37
24	7	314	CLA	C1D-ND	3.35	1.41	1.37
24	S	613	CLA	C1D-ND	3.35	1.41	1.37
24	BE	611	CLA	C1D-ND	3.35	1.41	1.37
23	G	609	CHL	OBD-CAD	3.35	1.28	1.22
24	AA	304	CLA	C1D-ND	3.35	1.41	1.37
24	2	403	CLA	C1D-ND	3.35	1.41	1.37
29	v	618	BCR	C30-C25	-3.35	1.49	1.53
23	9	609	CHL	MG-NA	-3.35	1.98	2.06
23	7	307	CHL	CHC-C4B	3.35	1.46	1.39
23	Y	310	CHL	OBD-CAD	3.35	1.28	1.22
23	BB	307	CHL	CHC-C4B	3.35	1.46	1.39
24	a	406	CLA	C4D-ND	-3.35	1.33	1.37
24	Au	602	CLA	C4D-ND	-3.35	1.33	1.37
23	Y	302	CHL	CHC-C4B	3.35	1.46	1.39
23	y	306	CHL	CHB-C1B	3.35	1.46	1.39
24	S	604	CLA	C1D-ND	3.35	1.41	1.37
23	Au	605	CHL	CHB-C1B	3.35	1.46	1.39
24	Y	304	CLA	C4D-ND	-3.35	1.33	1.37
24	d	401	CLA	C4D-ND	-3.34	1.33	1.37
23	r	606	CHL	CHC-C4B	3.34	1.46	1.39
24	g	613	CLA	C4B-NB	3.34	1.41	1.37
23	BB	307	CHL	CHD-C4C	3.34	1.46	1.39
24	1	505	CLA	C1D-ND	3.34	1.41	1.37
23	7	309	CHL	CHC-C4B	3.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	305	CLA	C4D-ND	-3.34	1.33	1.37
32	l	101	SQD	O47-C45	-3.34	1.38	1.46
23	s	601	CHL	CHB-C1B	3.34	1.46	1.39
23	AA	308	CHL	CHC-C4B	3.34	1.46	1.39
24	n	611	CLA	C4B-NB	3.34	1.41	1.37
24	B	606	CLA	C4B-NB	3.34	1.41	1.37
24	c	502	CLA	C1D-ND	3.34	1.41	1.37
24	BD	405	CLA	C1D-ND	3.34	1.41	1.37
23	BB	306	CHL	CHB-C1B	3.34	1.46	1.39
23	BJ	608	CHL	CHC-C4B	3.34	1.46	1.39
26	BJ	617	NEX	C10-C9	3.34	1.40	1.35
24	C	506	CLA	C4D-ND	-3.34	1.33	1.37
24	c	504	CLA	C4D-ND	-3.34	1.33	1.37
24	c	511	CLA	C4D-ND	-3.34	1.33	1.37
23	BB	306	CHL	OBD-CAD	3.34	1.28	1.22
23	AA	302	CHL	OBD-CAD	3.34	1.28	1.22
23	BV	605	CHL	CHB-C1B	3.34	1.46	1.39
24	v	614	CLA	C1D-ND	3.34	1.41	1.37
24	BF	509	CLA	C1D-ND	3.34	1.41	1.37
23	n	601	CHL	CHB-C1B	3.34	1.46	1.39
23	5	605	CHL	CHB-C1B	3.34	1.46	1.39
23	Y	307	CHL	CHC-C4B	3.34	1.46	1.39
24	v	613	CLA	C1D-ND	3.34	1.41	1.37
23	Au	607	CHL	CHC-C4B	3.34	1.46	1.39
23	A2	608	CHL	OBD-CAD	3.34	1.28	1.22
23	BB	309	CHL	OBD-CAD	3.33	1.28	1.22
24	BJ	613	CLA	C4B-NB	3.33	1.41	1.37
23	9	605	CHL	CHB-C1B	3.33	1.46	1.39
23	9	606	CHL	OBD-CAD	3.33	1.28	1.22
24	5	604	CLA	C3B-C4B	3.33	1.50	1.42
23	A2	605	CHL	OBD-CAD	3.33	1.28	1.22
24	BV	608	CLA	C4B-NB	3.33	1.41	1.37
23	5	609	CHL	OBD-CAD	3.33	1.28	1.22
26	n	617	NEX	C10-C9	3.33	1.40	1.35
24	n	613	CLA	C4B-NB	3.33	1.41	1.37
23	AA	307	CHL	CHC-C4B	3.33	1.46	1.39
25	AB	311	LUT	C32-C33	-3.33	1.38	1.45
23	y	302	CHL	CHB-C1B	3.33	1.46	1.39
24	7	304	CLA	C1D-ND	3.33	1.41	1.37
23	s	606	CHL	CHB-C1B	3.33	1.46	1.39
23	BV	606	CHL	CHB-C1B	3.33	1.46	1.39
24	N	604	CLA	C1D-ND	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C1D-ND	3.33	1.41	1.37
24	BB	304	CLA	C4D-ND	-3.33	1.33	1.37
23	BU	606	CHL	CHC-C4B	3.33	1.46	1.39
24	v	604	CLA	C1D-ND	3.33	1.41	1.37
32	A	413	SQD	O5-C1	3.33	1.50	1.41
24	A6	613	CLA	C1D-ND	3.33	1.41	1.37
24	N	612	CLA	C1D-ND	3.33	1.41	1.37
23	7	308	CHL	CHC-C4B	3.33	1.46	1.39
23	s	605	CHL	CHB-C1B	3.33	1.46	1.39
24	C	509	CLA	C1D-ND	3.33	1.41	1.37
24	B	608	CLA	C1D-ND	3.32	1.41	1.37
24	AA	314	CLA	C1D-ND	3.32	1.41	1.37
24	BE	614	CLA	C1D-ND	3.32	1.41	1.37
23	AA	307	CHL	CHB-C1B	3.32	1.46	1.39
23	9	608	CHL	CHC-C4B	3.32	1.46	1.39
23	0	608	CHL	CHB-C1B	3.32	1.46	1.39
23	6	609	CHL	MG-NA	-3.32	1.98	2.06
23	N	605	CHL	OBD-CAD	3.32	1.28	1.22
24	B	616	CLA	C4D-ND	-3.32	1.33	1.37
24	0	610	CLA	C4D-ND	-3.32	1.33	1.37
24	c	507	CLA	C4D-ND	-3.32	1.33	1.37
24	BB	315	CLA	C4D-ND	-3.32	1.33	1.37
24	Y	315	CLA	C1D-ND	3.32	1.41	1.37
23	G	601	CHL	CHC-C4B	3.32	1.46	1.39
24	G	611	CLA	C1D-ND	3.32	1.41	1.37
29	Av	101	BCR	C30-C25	-3.32	1.49	1.53
23	A6	607	CHL	CHB-C1B	3.32	1.46	1.39
23	Ba	306	CHL	CHB-C1B	3.32	1.46	1.39
24	6	611	CLA	C1D-ND	3.32	1.41	1.37
32	l	101	SQD	O47-C7	3.31	1.43	1.34
24	s	608	CLA	C4B-NB	3.31	1.41	1.37
23	AA	309	CHL	CHC-C4B	3.31	1.46	1.39
24	c	510	CLA	C1D-ND	3.31	1.41	1.37
24	1	512	CLA	C4D-ND	-3.31	1.33	1.37
25	AB	311	LUT	C30-C29	3.31	1.40	1.35
23	N	601	CHL	CHC-C4B	3.31	1.46	1.39
24	1	513	CLA	C1D-ND	3.31	1.41	1.37
24	BE	614	CLA	C4D-ND	-3.31	1.33	1.37
24	1	510	CLA	C4D-ND	-3.31	1.33	1.37
24	BU	603	CLA	C4D-ND	-3.31	1.33	1.37
23	8	306	CHL	CHB-C1B	3.31	1.46	1.39
24	c	507	CLA	C1D-ND	3.31	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BJ	604	CLA	C4B-NB	3.31	1.41	1.37
24	B	601	CLA	C4B-NB	3.31	1.41	1.37
24	A2	612	CLA	C4D-ND	-3.31	1.33	1.37
23	Y	310	CHL	CHC-C4B	3.31	1.46	1.39
24	C	502	CLA	C1D-ND	3.31	1.41	1.37
24	BE	615	CLA	C1D-ND	3.31	1.41	1.37
23	G	608	CHL	CHC-C4B	3.31	1.46	1.39
24	BE	609	CLA	C1D-ND	3.31	1.41	1.37
24	1	510	CLA	C1D-ND	3.31	1.41	1.37
23	BB	302	CHL	OBD-CAD	3.31	1.28	1.22
24	C	510	CLA	C1D-ND	3.31	1.41	1.37
25	AB	311	LUT	C14-C13	3.31	1.40	1.35
23	g	608	CHL	CHC-C4B	3.30	1.46	1.39
24	r	603	CLA	C4D-ND	-3.30	1.33	1.37
24	1	511	CLA	C4D-ND	-3.30	1.33	1.37
25	8	311	LUT	C10-C9	3.30	1.40	1.35
23	6	608	CHL	CHB-C1B	3.30	1.46	1.39
23	9	607	CHL	CHC-C4B	3.30	1.46	1.39
23	Au	608	CHL	CHC-C4B	3.30	1.46	1.39
29	BE	619	BCR	C1-C6	-3.30	1.49	1.53
24	G	602	CLA	C1D-ND	3.30	1.41	1.37
24	BQ	602	CLA	C4B-NB	3.30	1.41	1.37
23	6	609	CHL	C1B-NB	-3.30	1.33	1.37
24	A2	611	CLA	C1D-ND	3.30	1.41	1.37
24	BQ	613	CLA	C4B-NB	3.30	1.41	1.37
23	A2	601	CHL	CHC-C4B	3.30	1.46	1.39
23	7	307	CHL	CHB-C1B	3.30	1.46	1.39
24	S	609	CLA	C1D-ND	3.30	1.41	1.37
24	s	603	CLA	C4B-NB	3.30	1.41	1.37
24	7	314	CLA	C4D-ND	-3.30	1.33	1.37
24	AA	314	CLA	C4D-ND	-3.30	1.33	1.37
24	v	616	CLA	C4D-ND	-3.30	1.33	1.37
24	A2	604	CLA	C1D-ND	3.30	1.41	1.37
23	BV	601	CHL	CHB-C1B	3.30	1.46	1.39
24	v	615	CLA	C1D-ND	3.30	1.41	1.37
24	A6	609	CLA	C1D-ND	3.30	1.41	1.37
24	N	602	CLA	C4D-ND	-3.29	1.33	1.37
23	7	309	CHL	CHB-C1B	3.29	1.46	1.39
24	b	614	CLA	C1D-ND	3.29	1.41	1.37
24	g	603	CLA	C4B-NB	3.29	1.41	1.37
24	BJ	603	CLA	C4B-NB	3.29	1.41	1.37
24	1	502	CLA	C1D-ND	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	310	CLA	C4D-ND	-3.29	1.33	1.37
24	R	405	CLA	C4D-ND	-3.29	1.33	1.37
23	y	310	CHL	OBD-CAD	3.29	1.28	1.22
24	C	512	CLA	C1D-ND	3.29	1.41	1.37
24	v	601	CLA	C4B-NB	3.29	1.41	1.37
24	I	102	CLA	C4D-ND	-3.29	1.33	1.37
23	AB	306	CHL	CHB-C1B	3.29	1.46	1.39
24	AA	311	CLA	C4D-ND	-3.29	1.33	1.37
24	BF	514	CLA	C1D-ND	3.29	1.41	1.37
32	2	408	SQD	O5-C1	3.29	1.50	1.41
23	BB	309	CHL	CHB-C1B	3.29	1.46	1.39
24	Y	314	CLA	C4D-ND	-3.29	1.33	1.37
24	1	506	CLA	C4D-ND	-3.29	1.33	1.37
24	Y	313	CLA	C1D-ND	3.29	1.41	1.37
24	v	604	CLA	C4D-ND	-3.29	1.33	1.37
32	l	102	SQD	O5-C1	3.29	1.50	1.41
23	AA	302	CHL	CHB-C1B	3.29	1.46	1.39
32	D	406	SQD	O47-C7	3.29	1.43	1.34
24	C	503	CLA	C4D-ND	-3.29	1.33	1.37
23	N	609	CHL	OBD-CAD	3.28	1.28	1.22
24	n	603	CLA	C4B-NB	3.28	1.41	1.37
24	6	614	CLA	C1D-ND	3.28	1.41	1.37
24	a	405	CLA	C1D-ND	3.28	1.41	1.37
24	AA	311	CLA	C4B-NB	3.28	1.41	1.37
24	BV	604	CLA	C4B-NB	3.28	1.41	1.37
24	b	613	CLA	C4D-ND	-3.28	1.33	1.37
24	9	611	CLA	C4D-ND	-3.28	1.33	1.37
29	4	101	BCR	C30-C25	-3.28	1.49	1.53
23	AA	309	CHL	CHB-C1B	3.28	1.46	1.39
29	F	101	BCR	C30-C25	-3.28	1.49	1.53
24	b	613	CLA	C1D-ND	3.28	1.41	1.37
24	A2	610	CLA	C1D-ND	3.28	1.41	1.37
23	N	607	CHL	CHC-C4B	3.28	1.46	1.39
24	6	610	CLA	C4D-ND	-3.28	1.33	1.37
23	6	609	CHL	CHB-C1B	3.28	1.46	1.39
24	8	302	CLA	C1D-ND	3.28	1.41	1.37
24	AA	311	CLA	C1D-ND	3.28	1.41	1.37
24	1	513	CLA	C4D-ND	-3.28	1.33	1.37
24	9	604	CLA	C3B-C4B	3.28	1.50	1.42
23	9	609	CHL	OBD-CAD	3.28	1.28	1.22
24	0	614	CLA	C1D-ND	3.28	1.41	1.37
32	BO	102	SQD	O5-C1	3.28	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	v	608	CLA	C1D-ND	3.27	1.41	1.37
24	v	610	CLA	C1D-ND	3.27	1.41	1.37
23	Ba	302	CHL	CHB-C1B	3.27	1.46	1.39
24	A2	603	CLA	C4D-ND	-3.27	1.33	1.37
24	G	610	CLA	C1D-ND	3.27	1.41	1.37
24	Aw	102	CLA	C4D-ND	-3.27	1.33	1.37
24	C	507	CLA	C1D-ND	3.27	1.41	1.37
24	1	507	CLA	C1D-ND	3.27	1.41	1.37
24	N	603	CLA	C1D-ND	3.27	1.41	1.37
24	Au	610	CLA	C1D-ND	3.27	1.41	1.37
26	BB	318	NEX	C10-C9	3.27	1.40	1.35
24	g	611	CLA	C4B-NB	3.27	1.41	1.37
24	5	602	CLA	C4D-ND	-3.27	1.33	1.37
24	BD	410	CLA	C4D-ND	-3.27	1.33	1.37
24	y	305	CLA	C4B-NB	3.27	1.41	1.37
29	BE	619	BCR	C30-C25	-3.27	1.49	1.53
24	BF	514	CLA	C4D-ND	-3.27	1.33	1.37
25	8	311	LUT	C8-C9	-3.27	1.38	1.45
24	BB	313	CLA	C4D-ND	-3.27	1.33	1.37
23	AA	310	CHL	CHB-C1B	3.26	1.46	1.39
24	r	604	CLA	C1D-ND	3.26	1.41	1.37
24	AB	302	CLA	C1D-ND	3.26	1.41	1.37
24	A2	612	CLA	C1D-ND	3.26	1.41	1.37
24	BE	617	CLA	C4D-ND	-3.26	1.33	1.37
25	r	615	LUT	C34-C33	3.26	1.40	1.35
24	A6	611	CLA	C4D-ND	-3.26	1.33	1.37
24	Ba	311	CLA	C4D-ND	-3.26	1.33	1.37
24	c	514	CLA	C1D-ND	3.26	1.41	1.37
24	Au	603	CLA	C1D-ND	3.26	1.41	1.37
24	8	310	CLA	C4D-ND	-3.26	1.33	1.37
24	C	505	CLA	C4D-ND	-3.26	1.33	1.37
24	C	504	CLA	C1D-ND	3.26	1.41	1.37
24	AA	313	CLA	C1D-ND	3.26	1.41	1.37
24	b	614	CLA	C4D-ND	-3.26	1.33	1.37
24	9	602	CLA	C4D-ND	-3.26	1.33	1.37
24	C	512	CLA	C4D-ND	-3.26	1.33	1.37
24	C	503	CLA	C1D-ND	3.26	1.41	1.37
23	7	310	CHL	CHB-C1B	3.26	1.46	1.39
23	BB	310	CHL	CHC-C4B	3.26	1.46	1.39
24	BB	312	CLA	C1D-ND	3.26	1.41	1.37
24	Ba	304	CLA	C3B-C4B	3.26	1.50	1.42
24	A2	602	CLA	C4D-ND	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	C4D-ND	-3.26	1.33	1.37
29	H	101	BCR	C30-C25	-3.26	1.49	1.53
24	BB	315	CLA	C1D-ND	3.26	1.41	1.37
24	N	612	CLA	C4D-ND	-3.25	1.33	1.37
24	Au	610	CLA	C4D-ND	-3.25	1.33	1.37
25	BU	615	LUT	C34-C33	3.25	1.40	1.35
24	AA	313	CLA	C4B-NB	3.25	1.41	1.37
23	AB	307	CHL	CHB-C1B	3.25	1.46	1.39
24	G	603	CLA	C4D-ND	-3.25	1.33	1.37
24	A	406	CLA	C1D-ND	3.25	1.41	1.37
23	Au	601	CHL	CHC-C4B	3.25	1.46	1.39
24	BQ	614	CLA	C3B-C4B	3.25	1.50	1.42
24	1	506	CLA	C1D-ND	3.25	1.41	1.37
23	BJ	606	CHL	CHB-C1B	3.25	1.46	1.39
32	L	103	SQD	O47-C7	3.25	1.43	1.34
24	N	603	CLA	C4D-ND	-3.25	1.33	1.37
24	BJ	614	CLA	C4B-NB	3.25	1.41	1.37
24	1	505	CLA	C4D-ND	-3.25	1.33	1.37
25	r	615	LUT	C10-C9	3.25	1.40	1.35
24	1	509	CLA	C1D-ND	3.25	1.41	1.37
24	C	510	CLA	C4D-ND	-3.25	1.33	1.37
23	g	606	CHL	CHB-C1B	3.25	1.46	1.39
25	BU	615	LUT	C10-C9	3.25	1.40	1.35
24	Y	313	CLA	C4D-ND	-3.25	1.33	1.37
24	C	504	CLA	C4D-ND	-3.25	1.33	1.37
24	BQ	603	CLA	C4B-NB	3.24	1.41	1.37
24	5	611	CLA	C4D-ND	-3.24	1.33	1.37
23	BJ	605	CHL	CHB-C1B	3.24	1.46	1.39
24	Y	315	CLA	C4D-ND	-3.24	1.33	1.37
23	e	601	CHL	CHB-C1B	3.24	1.46	1.39
24	s	608	CLA	C4D-ND	-3.24	1.33	1.37
29	b	618	BCR	C30-C25	-3.24	1.49	1.53
24	N	610	CLA	C1D-ND	3.24	1.41	1.37
24	y	304	CLA	C3B-C4B	3.24	1.50	1.42
24	B	613	CLA	C4D-ND	-3.24	1.33	1.37
32	A1	101	SQD	O47-C7	3.24	1.43	1.34
24	v	613	CLA	C4D-ND	-3.24	1.33	1.37
24	C	508	CLA	C1D-ND	3.24	1.41	1.37
23	5	606	CHL	CHC-C4B	3.24	1.46	1.39
24	G	610	CLA	C4D-ND	-3.24	1.33	1.37
24	AB	309	CLA	C4B-NB	3.24	1.41	1.37
23	7	302	CHL	CHB-C1B	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	610	CLA	C3B-C4B	3.24	1.50	1.42
23	9	609	CHL	C1B-NB	-3.24	1.33	1.37
24	d	402	CLA	C4D-ND	-3.24	1.33	1.37
24	c	505	CLA	C4D-ND	-3.24	1.33	1.37
24	A6	610	CLA	C4D-ND	-3.24	1.33	1.37
24	BE	605	CLA	C4D-ND	-3.24	1.33	1.37
24	BQ	610	CLA	C4D-ND	-3.24	1.33	1.37
23	BQ	609	CHL	CHB-C1B	3.23	1.46	1.39
23	g	609	CHL	C1D-C2D	3.23	1.51	1.45
24	Y	312	CLA	C1D-ND	3.23	1.41	1.37
24	n	602	CLA	C4B-NB	3.23	1.41	1.37
24	C	506	CLA	C1D-ND	3.23	1.41	1.37
23	9	606	CHL	CHC-C4B	3.23	1.46	1.39
23	5	609	CHL	C4B-NB	-3.23	1.33	1.37
23	A2	607	CHL	CHC-C4B	3.23	1.46	1.39
24	b	605	CLA	C4D-ND	-3.23	1.33	1.37
24	Au	602	CLA	C1D-ND	3.23	1.41	1.37
32	D	406	SQD	O5-C1	3.23	1.50	1.41
24	A	410	CLA	C4D-ND	-3.23	1.33	1.37
24	A2	604	CLA	C4D-ND	-3.23	1.33	1.37
24	6	611	CLA	C4D-ND	-3.23	1.33	1.37
24	S	611	CLA	C4D-ND	-3.23	1.33	1.37
24	0	604	CLA	C4D-ND	-3.23	1.33	1.37
23	g	605	CHL	CHB-C1B	3.23	1.46	1.39
23	A6	601	CHL	CHB-C1B	3.23	1.46	1.39
24	B	606	CLA	C3B-C4B	3.23	1.50	1.42
24	v	606	CLA	C3B-C4B	3.23	1.50	1.42
24	n	614	CLA	C3B-C4B	3.23	1.50	1.42
24	y	313	CLA	C4B-NB	3.23	1.41	1.37
24	R	404	CLA	C4D-ND	-3.23	1.33	1.37
24	B	608	CLA	C4D-ND	-3.23	1.33	1.37
23	S	605	CHL	CHB-C1B	3.23	1.46	1.39
23	A6	605	CHL	CHB-C1B	3.23	1.46	1.39
24	6	613	CLA	C1D-ND	3.23	1.41	1.37
24	Ba	313	CLA	C4B-NB	3.23	1.41	1.37
24	G	612	CLA	C4D-ND	-3.23	1.33	1.37
23	n	609	CHL	CHB-C1B	3.22	1.46	1.39
24	0	610	CLA	C1D-ND	3.22	1.41	1.37
32	a	412	SQD	O47-C7	3.22	1.43	1.34
24	g	612	CLA	C3B-C4B	3.22	1.50	1.42
38	a	408	PHO	C4D-CHA	3.22	1.44	1.39
24	R	409	CLA	C4D-ND	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4D-ND	-3.22	1.33	1.37
24	B	615	CLA	C4D-ND	-3.22	1.33	1.37
23	0	609	CHL	OBD-CAD	3.22	1.28	1.22
24	Ba	315	CLA	C4D-ND	-3.22	1.33	1.37
24	BV	603	CLA	C4B-NB	3.22	1.41	1.37
23	G	608	CHL	CHB-C1B	3.22	1.46	1.39
24	Ba	305	CLA	C4B-NB	3.22	1.41	1.37
23	BU	613	CHL	CHB-C1B	3.22	1.46	1.39
24	8	310	CLA	C4B-NB	3.22	1.41	1.37
24	a	406	CLA	C1D-ND	3.22	1.41	1.37
23	Y	308	CHL	CHC-C4B	3.22	1.46	1.39
23	BH	601	CHL	CHB-C1B	3.22	1.46	1.39
24	c	505	CLA	C1D-ND	3.22	1.41	1.37
24	BB	313	CLA	C1D-ND	3.22	1.41	1.37
24	Au	612	CLA	C4D-ND	-3.22	1.33	1.37
23	AA	302	CHL	C1D-C2D	3.22	1.51	1.45
26	5	617	NEX	C10-C9	3.21	1.40	1.35
24	N	604	CLA	C4D-ND	-3.21	1.33	1.37
32	2	408	SQD	O47-C7	3.21	1.43	1.34
23	BU	605	CHL	CHB-C1B	3.21	1.46	1.39
24	BQ	604	CLA	C4B-NB	3.21	1.41	1.37
23	0	601	CHL	CHB-C1B	3.21	1.46	1.39
24	BJ	611	CLA	C4B-NB	3.21	1.41	1.37
24	Y	304	CLA	C1D-ND	3.21	1.41	1.37
24	g	602	CLA	C4B-NB	3.21	1.41	1.37
24	BF	507	CLA	C1D-ND	3.21	1.41	1.37
23	N	606	CHL	CHB-C1B	3.21	1.46	1.39
24	5	612	CLA	C4D-ND	-3.21	1.33	1.37
24	BF	504	CLA	C1D-ND	3.21	1.41	1.37
23	S	606	CHL	CHB-C1B	3.21	1.46	1.39
24	BQ	612	CLA	C4B-NB	3.21	1.41	1.37
24	BF	505	CLA	C4D-ND	-3.21	1.33	1.37
24	BF	506	CLA	C4D-ND	-3.21	1.33	1.37
24	BB	305	CLA	C4D-ND	-3.20	1.33	1.37
24	1	504	CLA	C4D-ND	-3.20	1.33	1.37
23	g	608	CHL	CHB-C1B	3.20	1.46	1.39
38	a	409	PHO	C1D-C2D	3.20	1.43	1.39
23	BJ	609	CHL	C1D-C2D	3.20	1.51	1.45
32	BD	412	SQD	O47-C7	3.20	1.43	1.34
24	g	610	CLA	C4B-NB	3.20	1.41	1.37
23	r	613	CHL	CHB-C1B	3.20	1.46	1.39
24	c	506	CLA	C4D-ND	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C4D-ND	-3.20	1.33	1.37
24	r	608	CLA	C1D-ND	3.20	1.41	1.37
23	BJ	608	CHL	CHB-C1B	3.20	1.46	1.39
24	2	403	CLA	C4D-ND	-3.20	1.33	1.37
24	Au	611	CLA	C4D-ND	-3.20	1.33	1.37
23	Au	608	CHL	CHB-C1B	3.20	1.46	1.39
23	n	605	CHL	CHB-C1B	3.20	1.46	1.39
23	AA	302	CHL	C3D-C2D	3.20	1.47	1.39
29	h	101	BCR	C30-C25	-3.20	1.49	1.53
24	BE	610	CLA	C4B-NB	3.20	1.41	1.37
24	D	402	CLA	C4D-ND	-3.20	1.33	1.37
24	y	311	CLA	C4D-ND	-3.20	1.33	1.37
23	AA	310	CHL	C4B-NB	-3.20	1.33	1.37
24	BE	602	CLA	C4B-NB	3.20	1.41	1.37
24	N	611	CLA	C4D-ND	-3.19	1.33	1.37
24	A6	609	CLA	C4D-ND	-3.19	1.33	1.37
23	N	605	CHL	CHB-C1B	3.19	1.46	1.39
23	7	302	CHL	C1D-C2D	3.19	1.51	1.45
23	6	601	CHL	CHB-C1B	3.19	1.46	1.39
23	A2	609	CHL	OBD-CAD	3.19	1.28	1.22
23	A2	605	CHL	CHB-C1B	3.19	1.46	1.39
24	R	406	CLA	C4D-ND	-3.19	1.33	1.37
24	0	603	CLA	C1D-ND	3.19	1.41	1.37
24	C	513	CLA	C4D-ND	-3.19	1.33	1.37
23	BB	308	CHL	CHC-C4B	3.19	1.46	1.39
24	c	503	CLA	C1D-ND	3.19	1.41	1.37
24	BE	609	CLA	C4D-ND	-3.19	1.33	1.37
25	r	615	LUT	C8-C9	-3.19	1.39	1.45
26	G	617	NEX	C10-C9	3.19	1.40	1.35
23	N	605	CHL	CHC-C4B	3.19	1.46	1.39
24	a	410	CLA	C4D-ND	-3.19	1.33	1.37
24	BG	402	CLA	C4D-ND	-3.19	1.33	1.37
24	Ba	305	CLA	C4D-ND	-3.19	1.33	1.37
23	Au	601	CHL	CHB-C1B	3.19	1.46	1.39
24	7	313	CLA	C4B-NB	3.19	1.41	1.37
24	A2	611	CLA	C4D-ND	-3.18	1.33	1.37
23	Au	607	CHL	CHB-C1B	3.18	1.46	1.39
24	BV	602	CLA	C4B-NB	3.18	1.41	1.37
23	6	609	CHL	OBD-CAD	3.18	1.28	1.22
24	BJ	612	CLA	C3B-C4B	3.18	1.50	1.42
24	7	313	CLA	C4D-ND	-3.18	1.33	1.37
25	BU	615	LUT	C8-C9	-3.18	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	617	NEX	C10-C9	3.18	1.40	1.35
24	n	612	CLA	C4B-NB	3.18	1.41	1.37
24	v	615	CLA	C4D-ND	-3.18	1.33	1.37
24	s	612	CLA	C4B-NB	3.18	1.41	1.37
24	9	614	CLA	C4B-NB	3.18	1.41	1.37
24	BV	612	CLA	C4B-NB	3.18	1.41	1.37
23	7	310	CHL	C4B-NB	-3.18	1.33	1.37
24	y	303	CLA	C4B-NB	3.18	1.41	1.37
23	8	307	CHL	CHB-C1B	3.18	1.46	1.39
24	8	309	CLA	C4B-NB	3.18	1.41	1.37
24	s	604	CLA	C4B-NB	3.18	1.41	1.37
24	1	504	CLA	C1D-ND	3.18	1.41	1.37
23	BQ	605	CHL	CHB-C1B	3.17	1.46	1.39
23	r	605	CHL	C2C-C3C	3.17	1.43	1.36
24	A6	613	CLA	C4D-ND	-3.17	1.33	1.37
32	A	413	SQD	O47-C7	3.17	1.43	1.34
24	v	608	CLA	C4D-ND	-3.17	1.33	1.37
24	Au	603	CLA	C4D-ND	-3.17	1.33	1.37
23	r	605	CHL	CHB-C1B	3.17	1.46	1.39
24	BU	603	CLA	C1D-ND	3.17	1.41	1.37
23	6	606	CHL	CHC-C4B	3.17	1.46	1.39
23	A6	606	CHL	CHB-C1B	3.17	1.46	1.39
24	N	602	CLA	C1D-ND	3.17	1.41	1.37
24	Ba	314	CLA	C4B-NB	3.17	1.41	1.37
29	v	619	BCR	C30-C25	-3.17	1.49	1.53
24	b	617	CLA	C4D-ND	-3.17	1.33	1.37
24	A2	613	CLA	C4D-ND	-3.17	1.33	1.37
24	0	611	CLA	C1D-ND	3.17	1.41	1.37
29	BK	101	BCR	C30-C25	-3.17	1.49	1.53
24	7	311	CLA	C4D-ND	-3.17	1.33	1.37
24	g	614	CLA	C4B-NB	3.17	1.41	1.37
28	9	619	XAT	O24-C25	-3.17	1.41	1.46
23	A2	601	CHL	CHB-C1B	3.17	1.46	1.39
24	Y	305	CLA	C4D-ND	-3.17	1.33	1.37
23	A2	605	CHL	CHC-C4B	3.17	1.46	1.39
24	C	508	CLA	C4D-ND	-3.16	1.33	1.37
23	0	606	CHL	CHC-C4B	3.16	1.46	1.39
23	BU	606	CHL	C1B-NB	-3.16	1.33	1.37
24	c	511	CLA	C1D-ND	3.16	1.41	1.37
24	v	609	CLA	C4D-ND	-3.16	1.33	1.37
26	s	616	NEX	C10-C9	3.16	1.40	1.35
24	R	405	CLA	C1D-ND	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Au	613	CLA	C4D-ND	-3.16	1.33	1.37
24	BB	314	CLA	C1D-ND	3.16	1.41	1.37
23	S	601	CHL	CHB-C1B	3.16	1.46	1.39
23	Ba	310	CHL	C3D-C2D	3.16	1.47	1.39
24	5	603	CLA	C1D-ND	3.16	1.41	1.37
24	BE	616	CLA	C4D-ND	-3.16	1.33	1.37
38	BD	408	PHO	C4D-CHA	3.16	1.44	1.39
29	b	619	BCR	C30-C25	-3.16	1.49	1.53
24	5	611	CLA	C4B-NB	3.16	1.41	1.37
24	S	609	CLA	C4D-ND	-3.16	1.33	1.37
24	v	605	CLA	C4D-ND	-3.16	1.33	1.37
23	N	601	CHL	CHB-C1B	3.16	1.46	1.39
23	BB	310	CHL	OBD-CAD	3.16	1.27	1.22
24	6	604	CLA	C1D-ND	3.15	1.41	1.37
24	n	604	CLA	C4B-NB	3.15	1.41	1.37
24	BJ	610	CLA	C4B-NB	3.15	1.41	1.37
24	AA	313	CLA	C3B-C4B	3.15	1.50	1.42
29	BI	101	BCR	C30-C25	-3.15	1.49	1.53
24	Y	314	CLA	C1D-ND	3.15	1.41	1.37
23	5	608	CHL	CHB-C1B	3.15	1.46	1.39
23	N	607	CHL	CHB-C1B	3.15	1.46	1.39
24	r	611	CLA	C1D-ND	3.15	1.41	1.37
24	AB	301	CLA	C4D-ND	-3.15	1.33	1.37
24	s	604	CLA	C3B-C4B	3.15	1.50	1.42
24	1	503	CLA	C1D-ND	3.15	1.41	1.37
23	AA	310	CHL	MG-NA	-3.15	1.98	2.06
25	8	311	LUT	C34-C33	3.15	1.40	1.35
32	R	411	SQD	O47-C7	3.15	1.43	1.34
24	r	603	CLA	C1D-ND	3.15	1.41	1.37
38	BD	409	PHO	C1D-C2D	3.15	1.43	1.39
23	7	302	CHL	C3D-C2D	3.15	1.47	1.39
24	Ba	312	CLA	C4D-ND	-3.15	1.33	1.37
23	s	607	CHL	C3D-C2D	3.15	1.47	1.39
24	v	610	CLA	C4D-ND	-3.15	1.33	1.37
24	b	602	CLA	C4B-NB	3.15	1.41	1.37
23	BU	605	CHL	C2C-C3C	3.15	1.43	1.36
23	BV	607	CHL	C3D-C2D	3.15	1.47	1.39
24	b	616	CLA	C4D-ND	-3.15	1.33	1.37
24	c	502	CLA	C4D-ND	-3.15	1.33	1.37
24	v	611	CLA	C4D-ND	-3.15	1.33	1.37
24	BU	604	CLA	C4D-ND	-3.15	1.33	1.37
24	N	614	CLA	C3B-C4B	3.15	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BF	510	CLA	C1D-ND	3.15	1.41	1.37
24	BE	607	CLA	C3B-C4B	3.14	1.50	1.42
32	d	406	SQD	O47-C7	3.14	1.43	1.34
32	BG	406	SQD	O47-C7	3.14	1.43	1.34
24	b	610	CLA	C4B-NB	3.14	1.41	1.37
29	Ay	101	BCR	C30-C25	-3.14	1.49	1.53
23	6	607	CHL	CHC-C4B	3.14	1.46	1.39
26	BB	320	NEX	C10-C9	3.14	1.39	1.35
24	Ba	303	CLA	C4B-NB	3.14	1.41	1.37
24	b	609	CLA	C4D-ND	-3.14	1.33	1.37
24	c	508	CLA	C1D-ND	3.14	1.41	1.37
24	9	611	CLA	C4B-NB	3.14	1.41	1.37
24	s	602	CLA	C4B-NB	3.14	1.41	1.37
24	1	508	CLA	C1D-ND	3.14	1.41	1.37
24	BU	608	CLA	C1D-ND	3.14	1.41	1.37
24	A2	602	CLA	C1D-ND	3.14	1.41	1.37
24	y	312	CLA	C4D-ND	-3.14	1.33	1.37
24	r	604	CLA	C4D-ND	-3.14	1.33	1.37
24	n	610	CLA	C4D-ND	-3.14	1.33	1.37
24	BV	613	CLA	C4D-ND	-3.14	1.33	1.37
24	7	315	CLA	C4B-NB	3.14	1.41	1.37
24	BF	503	CLA	C1D-ND	3.13	1.41	1.37
23	8	305	CHL	CHB-C1B	3.13	1.46	1.39
23	A2	606	CHL	CHB-C1B	3.13	1.46	1.39
24	S	610	CLA	C4D-ND	-3.13	1.33	1.37
23	BQ	607	CHL	CHB-C1B	3.13	1.46	1.39
24	G	613	CLA	C4D-ND	-3.13	1.33	1.37
24	BE	603	CLA	C4D-ND	-3.13	1.33	1.37
38	A	408	PHO	C4D-CHA	3.13	1.44	1.39
24	S	610	CLA	C4B-NB	3.13	1.41	1.37
28	8	312	XAT	O4-C5	-3.13	1.41	1.46
24	B	610	CLA	C4D-ND	-3.13	1.33	1.37
24	9	612	CLA	C4D-ND	-3.13	1.33	1.37
23	BJ	601	CHL	CHB-C1B	3.13	1.46	1.39
24	A2	603	CLA	C1D-ND	3.13	1.41	1.37
24	c	513	CLA	C1D-ND	3.13	1.41	1.37
24	BF	502	CLA	C4D-ND	-3.13	1.33	1.37
24	b	611	CLA	C4D-ND	-3.13	1.33	1.37
24	c	509	CLA	C4D-ND	-3.13	1.33	1.37
24	BF	509	CLA	C4D-ND	-3.13	1.33	1.37
24	B	605	CLA	C4D-ND	-3.13	1.33	1.37
24	r	612	CLA	C1D-ND	3.13	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	602	CLA	C1D-ND	3.13	1.41	1.37
23	g	601	CHL	CHB-C1B	3.13	1.46	1.39
24	A	405	CLA	C4D-ND	-3.13	1.33	1.37
23	r	606	CHL	OBD-CAD	3.13	1.27	1.22
24	BD	406	CLA	C1D-ND	3.13	1.41	1.37
23	y	310	CHL	C3D-C2D	3.13	1.47	1.39
25	6	615	LUT	C14-C13	3.12	1.39	1.35
25	AB	311	LUT	C8-C9	-3.12	1.39	1.45
24	BJ	602	CLA	C4B-NB	3.12	1.41	1.37
23	Au	609	CHL	CHC-C4B	3.12	1.46	1.39
27	BU	617	LHG	O7-C5	-3.12	1.38	1.46
28	5	619	XAT	O24-C25	-3.12	1.41	1.46
25	0	615	LUT	C8-C9	-3.12	1.39	1.45
23	AB	305	CHL	CHB-C1B	3.12	1.46	1.39
23	G	601	CHL	CHB-C1B	3.12	1.46	1.39
24	B	614	CLA	C4D-ND	-3.12	1.33	1.37
24	b	608	CLA	C4D-ND	-3.12	1.33	1.37
24	BF	508	CLA	C1D-ND	3.12	1.41	1.37
24	B	609	CLA	C4D-ND	-3.12	1.33	1.37
24	s	613	CLA	C4D-ND	-3.12	1.33	1.37
24	6	603	CLA	C1D-ND	3.12	1.41	1.37
24	b	610	CLA	C1D-ND	3.12	1.41	1.37
29	B	619	BCR	C30-C25	-3.12	1.49	1.53
23	AA	310	CHL	C1B-NB	-3.12	1.33	1.37
24	y	314	CLA	C4B-NB	3.12	1.41	1.37
24	BU	611	CLA	C1D-ND	3.12	1.41	1.37
28	AB	312	XAT	O4-C5	-3.12	1.41	1.46
23	0	609	CHL	MG-NA	-3.12	1.98	2.06
29	BE	620	BCR	C30-C25	-3.12	1.49	1.53
24	1	512	CLA	C1D-ND	3.12	1.41	1.37
24	BE	612	CLA	C4D-ND	-3.12	1.33	1.37
29	f	101	BCR	C30-C25	-3.12	1.49	1.53
24	C	502	CLA	C4D-ND	-3.12	1.33	1.37
24	1	508	CLA	C4D-ND	-3.12	1.33	1.37
24	r	601	CLA	C1D-ND	3.12	1.41	1.37
23	BU	607	CHL	CHC-C4B	3.12	1.46	1.39
23	r	605	CHL	CHC-C1C	3.11	1.44	1.38
24	BV	608	CLA	C4D-ND	-3.11	1.33	1.37
23	7	306	CHL	C3D-C2D	3.11	1.47	1.39
24	BF	511	CLA	C1D-ND	3.11	1.41	1.37
24	v	602	CLA	C4D-ND	-3.11	1.33	1.37
26	Au	617	NEX	C10-C9	3.11	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BE	601	BCR	C30-C25	-3.11	1.49	1.53
24	9	603	CLA	C1D-ND	3.11	1.41	1.37
23	7	310	CHL	MG-NA	-3.11	1.98	2.06
23	r	606	CHL	C1B-NB	-3.11	1.34	1.37
24	BQ	610	CLA	C4B-NB	3.11	1.41	1.37
24	AA	315	CLA	C4B-NB	3.11	1.41	1.37
24	BU	614	CLA	C4B-NB	3.11	1.41	1.37
24	B	611	CLA	C4D-ND	-3.11	1.33	1.37
23	Ba	308	CHL	CHB-C1B	3.11	1.46	1.39
24	S	604	CLA	C4D-ND	-3.11	1.33	1.37
24	y	315	CLA	C4D-ND	-3.11	1.33	1.37
24	AA	313	CLA	C4D-ND	-3.11	1.33	1.37
24	BB	311	CLA	C1D-ND	3.11	1.41	1.37
24	8	301	CLA	C4D-ND	-3.11	1.33	1.37
24	A6	604	CLA	C4D-ND	-3.11	1.33	1.37
24	b	607	CLA	C3B-C4B	3.11	1.50	1.42
23	AA	306	CHL	C1D-C2D	3.11	1.51	1.45
24	5	614	CLA	C4B-NB	3.11	1.41	1.37
23	N	609	CHL	CHB-C1B	3.11	1.46	1.39
26	N	617	NEX	C10-C9	3.11	1.39	1.35
24	b	603	CLA	C4B-NB	3.11	1.41	1.37
23	r	607	CHL	CHC-C4B	3.11	1.46	1.39
38	R	407	PHO	C4D-CHA	3.11	1.44	1.39
23	A2	609	CHL	CHB-C1B	3.10	1.46	1.39
23	A2	607	CHL	CHB-C1B	3.10	1.46	1.39
24	r	614	CLA	C4B-NB	3.10	1.41	1.37
24	B	602	CLA	C4D-ND	-3.10	1.33	1.37
24	1	502	CLA	C4D-ND	-3.10	1.33	1.37
23	7	310	CHL	C1B-NB	-3.10	1.34	1.37
24	A2	614	CLA	C3B-C4B	3.10	1.50	1.42
24	b	615	CLA	C4D-ND	-3.10	1.33	1.37
24	6	602	CLA	C1D-ND	3.10	1.41	1.37
24	S	603	CLA	C4B-NB	3.10	1.41	1.37
24	9	613	CLA	C4D-ND	-3.10	1.33	1.37
24	Y	311	CLA	C1D-ND	3.10	1.41	1.37
24	a	405	CLA	C4D-ND	-3.10	1.33	1.37
24	BE	615	CLA	C4D-ND	-3.10	1.33	1.37
24	a	407	CLA	C4D-ND	-3.10	1.33	1.37
24	v	606	CLA	C4D-ND	-3.10	1.33	1.37
24	v	607	CLA	C4D-ND	-3.10	1.33	1.37
24	A2	614	CLA	C4D-ND	-3.09	1.33	1.37
24	BD	407	CLA	C4D-ND	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	310	CHL	CHB-C1B	3.09	1.46	1.39
24	AB	309	CLA	C4D-ND	-3.09	1.33	1.37
24	BF	506	CLA	C1D-ND	3.09	1.41	1.37
24	b	610	CLA	C4D-ND	-3.09	1.33	1.37
23	0	609	CHL	C1B-NB	-3.09	1.34	1.37
23	y	308	CHL	CHB-C1B	3.09	1.46	1.39
23	9	608	CHL	CHB-C1B	3.09	1.46	1.39
24	5	604	CLA	C1D-ND	3.09	1.41	1.37
23	G	607	CHL	CHB-C1B	3.09	1.46	1.39
24	D	402	CLA	C4B-NB	3.09	1.41	1.37
24	BE	613	CLA	C1D-ND	3.09	1.41	1.37
23	n	601	CHL	C3D-C2D	3.09	1.47	1.39
24	b	612	CLA	C4D-ND	-3.09	1.33	1.37
23	Y	308	CHL	CHB-C1B	3.09	1.46	1.39
23	BJ	609	CHL	C3D-C2D	3.09	1.47	1.39
24	s	611	CLA	C4B-NB	3.09	1.41	1.37
24	B	606	CLA	C4D-ND	-3.09	1.33	1.37
24	C	511	CLA	C4D-ND	-3.09	1.33	1.37
24	AA	315	CLA	C4D-ND	-3.09	1.33	1.37
23	7	306	CHL	C1D-C2D	3.09	1.51	1.45
32	L	101	SQD	O5-C1	3.09	1.49	1.41
23	BQ	601	CHL	C3D-C2D	3.09	1.47	1.39
24	Ba	315	CLA	C4B-NB	3.09	1.41	1.37
24	BE	606	CLA	C4B-NB	3.08	1.41	1.37
24	Ba	311	CLA	C4B-NB	3.08	1.41	1.37
29	b	620	BCR	C30-C25	-3.08	1.49	1.53
24	Ba	314	CLA	C4D-ND	-3.08	1.33	1.37
23	g	609	CHL	C3D-C2D	3.08	1.47	1.39
38	R	408	PHO	C1D-C2D	3.08	1.43	1.39
24	BJ	602	CLA	C4D-ND	-3.08	1.33	1.37
24	c	505	CLA	C4B-NB	3.08	1.41	1.37
24	BF	513	CLA	C1D-ND	3.08	1.41	1.37
24	BE	611	CLA	C4D-ND	-3.08	1.33	1.37
23	n	607	CHL	CHB-C1B	3.08	1.46	1.39
24	y	305	CLA	C4D-ND	-3.08	1.33	1.37
25	s	614	LUT	C8-C9	-3.07	1.39	1.45
25	0	615	LUT	C28-C29	-3.07	1.39	1.45
24	N	613	CLA	C4D-ND	-3.07	1.33	1.37
24	BF	512	CLA	C4D-ND	-3.07	1.33	1.37
24	6	610	CLA	C3B-C4B	3.07	1.50	1.42
24	B	607	CLA	C4D-ND	-3.07	1.33	1.37
24	S	613	CLA	C4D-ND	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	609	CLA	C3B-C4B	3.07	1.49	1.42
23	s	601	CHL	C3D-C2D	3.07	1.47	1.39
23	AA	306	CHL	C3D-C2D	3.07	1.47	1.39
24	S	604	CLA	C4B-NB	3.07	1.41	1.37
24	n	611	CLA	C4D-ND	-3.07	1.33	1.37
24	r	610	CLA	C1D-ND	3.07	1.41	1.37
23	BU	606	CHL	OBD-CAD	3.07	1.27	1.22
24	s	610	CLA	C4B-NB	3.07	1.41	1.37
24	c	506	CLA	C1D-ND	3.07	1.41	1.37
23	BB	310	CHL	CHB-C1B	3.07	1.46	1.39
24	n	603	CLA	C4D-ND	-3.07	1.33	1.37
24	2	402	CLA	C1D-ND	3.07	1.41	1.37
24	5	613	CLA	C4D-ND	-3.07	1.33	1.37
24	BE	602	CLA	C4D-ND	-3.06	1.33	1.37
24	y	311	CLA	C4B-NB	3.06	1.41	1.37
24	BV	610	CLA	C4B-NB	3.06	1.41	1.37
23	r	606	CHL	CHB-C1B	3.06	1.46	1.39
24	n	612	CLA	C4D-ND	-3.06	1.33	1.37
24	BQ	603	CLA	C4D-ND	-3.06	1.33	1.37
24	G	612	CLA	C4B-NB	3.06	1.41	1.37
29	BN	101	BCR	C30-C25	-3.06	1.49	1.53
24	s	609	CLA	C4B-NB	3.06	1.41	1.37
29	K	101	BCR	C30-C25	-3.06	1.49	1.53
24	D	401	CLA	C1D-ND	3.06	1.41	1.37
24	N	614	CLA	C4D-ND	-3.06	1.33	1.37
24	BU	604	CLA	C1D-ND	3.06	1.41	1.37
26	A6	616	NEX	C10-C9	3.06	1.39	1.35
24	b	606	CLA	C4D-ND	-3.06	1.33	1.37
24	AB	302	CLA	C4B-NB	3.05	1.41	1.37
25	6	615	LUT	C34-C33	3.05	1.39	1.35
24	BU	610	CLA	C1D-ND	3.05	1.41	1.37
24	y	313	CLA	C3B-C4B	3.05	1.49	1.42
24	b	606	CLA	C4B-NB	3.05	1.41	1.37
33	f	102	HEM	CAC-C3C	3.05	1.55	1.47
24	7	311	CLA	C4B-NB	3.05	1.41	1.37
24	B	615	CLA	C4B-NB	3.05	1.41	1.37
24	A6	612	CLA	C4D-ND	-3.05	1.33	1.37
24	BE	610	CLA	C1D-ND	3.05	1.41	1.37
24	s	611	CLA	C4D-ND	-3.05	1.33	1.37
25	A2	615	LUT	C8-C9	-3.05	1.39	1.45
24	AA	312	CLA	C4D-ND	-3.05	1.33	1.37
24	y	315	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	602	CLA	C4D-ND	-3.05	1.33	1.37
24	BE	606	CLA	C4D-ND	-3.05	1.33	1.37
24	Ba	303	CLA	C4D-ND	-3.05	1.33	1.37
24	S	603	CLA	C4D-ND	-3.05	1.33	1.37
24	BD	405	CLA	C4D-ND	-3.05	1.33	1.37
24	BE	608	CLA	C4D-ND	-3.05	1.33	1.37
24	S	609	CLA	C4B-NB	3.05	1.41	1.37
24	B	609	CLA	C1D-ND	3.04	1.41	1.37
24	b	607	CLA	C4D-ND	-3.04	1.33	1.37
23	Y	302	CHL	CHB-C1B	3.04	1.46	1.39
24	7	304	CLA	C4B-NB	3.04	1.41	1.37
24	AA	304	CLA	C4B-NB	3.04	1.41	1.37
24	BV	602	CLA	C4D-ND	-3.04	1.33	1.37
24	v	614	CLA	C4D-ND	-3.04	1.33	1.37
24	G	614	CLA	C4B-NB	3.04	1.41	1.37
23	9	606	CHL	CHB-C1B	3.04	1.46	1.39
24	y	314	CLA	C4D-ND	-3.04	1.33	1.37
24	AB	310	CLA	C4B-NB	3.04	1.41	1.37
24	9	604	CLA	C1D-ND	3.04	1.41	1.37
24	c	502	CLA	C3B-C4B	3.04	1.49	1.42
24	AB	308	CLA	C3B-C4B	3.04	1.49	1.42
33	BI	102	HEM	CAC-C3C	3.04	1.55	1.47
29	v	622	BCR	C30-C25	-3.04	1.49	1.53
24	Au	604	CLA	C4D-ND	-3.04	1.33	1.37
23	BB	308	CHL	CHB-C1B	3.04	1.46	1.39
24	v	609	CLA	C1D-ND	3.04	1.41	1.37
33	BI	102	HEM	CAB-C3B	3.04	1.55	1.47
24	BJ	612	CLA	C4D-ND	-3.04	1.33	1.37
24	A6	609	CLA	C3B-C4B	3.04	1.49	1.42
25	7	316	LUT	C8-C9	-3.04	1.39	1.45
24	A6	603	CLA	C4B-NB	3.03	1.41	1.37
24	c	512	CLA	C4D-ND	-3.03	1.33	1.37
24	A6	608	CLA	C4D-ND	-3.03	1.33	1.37
24	Y	304	CLA	C4B-NB	3.03	1.41	1.37
24	8	302	CLA	C4B-NB	3.03	1.41	1.37
24	A6	610	CLA	C4B-NB	3.03	1.41	1.37
33	F	102	HEM	CAC-C3C	3.03	1.55	1.47
24	7	305	CLA	C4B-NB	3.03	1.41	1.37
33	f	102	HEM	CAB-C3B	3.03	1.55	1.47
25	y	316	LUT	C8-C9	-3.03	1.39	1.45
24	S	612	CLA	C4B-NB	3.03	1.41	1.37
24	7	312	CLA	C4D-ND	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BV	601	CHL	C3D-C2D	3.03	1.47	1.39
24	BQ	611	CLA	C4D-ND	-3.03	1.33	1.37
24	g	614	CLA	C4D-ND	-3.03	1.33	1.37
24	BU	601	CLA	C1D-ND	3.03	1.41	1.37
27	r	618	LHG	O7-C5	-3.03	1.39	1.46
23	0	601	CHL	C3D-C2D	3.03	1.47	1.39
28	BU	616	XAT	O24-C25	-3.02	1.41	1.46
23	Au	606	CHL	CHB-C1B	3.02	1.46	1.39
24	g	613	CLA	C4D-ND	-3.02	1.33	1.37
24	y	303	CLA	C4D-ND	-3.02	1.33	1.37
24	BB	304	CLA	C1D-ND	3.02	1.41	1.37
23	9	609	CHL	C3D-C2D	3.02	1.47	1.39
24	S	612	CLA	C4D-ND	-3.02	1.33	1.37
23	g	607	CHL	CHB-C1B	3.02	1.46	1.39
24	8	309	CLA	C4D-ND	-3.02	1.33	1.37
24	BV	611	CLA	C4D-ND	-3.02	1.33	1.37
23	G	606	CHL	CHB-C1B	3.02	1.46	1.39
24	A6	604	CLA	C4B-NB	3.02	1.41	1.37
24	BE	609	CLA	C4B-NB	3.02	1.41	1.37
38	A	408	PHO	CMC-C2C	-3.02	1.45	1.50
24	d	402	CLA	C4B-NB	3.02	1.41	1.37
25	BU	615	LUT	C30-C29	3.02	1.39	1.35
24	BV	610	CLA	C4D-ND	-3.01	1.33	1.37
24	7	315	CLA	C4D-ND	-3.01	1.33	1.37
24	y	304	CLA	C4D-ND	-3.01	1.33	1.37
24	BE	603	CLA	C4B-NB	3.01	1.41	1.37
24	A6	603	CLA	C4D-ND	-3.01	1.33	1.37
25	A6	615	LUT	C8-C9	-3.01	1.39	1.45
24	BV	609	CLA	C4D-ND	-3.01	1.33	1.37
24	A6	608	CLA	C4B-NB	3.01	1.41	1.37
24	b	604	CLA	C4D-ND	-3.01	1.33	1.37
25	r	615	LUT	C30-C29	3.01	1.39	1.35
24	Y	315	CLA	C4B-NB	3.01	1.41	1.37
24	7	312	CLA	C4B-NB	3.01	1.41	1.37
24	2	403	CLA	C4B-NB	3.01	1.41	1.37
24	BE	611	CLA	C4B-NB	3.01	1.41	1.37
23	G	609	CHL	C3D-C2D	3.01	1.47	1.39
23	Au	609	CHL	CHB-C1B	3.01	1.46	1.39
24	BU	608	CLA	C4B-NB	3.01	1.41	1.37
29	b	601	BCR	C30-C25	-3.01	1.49	1.53
24	g	602	CLA	C4D-ND	-3.01	1.33	1.37
24	BE	610	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BU	615	LUT	C32-C33	-3.01	1.39	1.45
33	4	102	HEM	CAC-C3C	3.01	1.55	1.47
24	C	502	CLA	C3B-C4B	3.01	1.49	1.42
24	Ba	313	CLA	C3B-C4B	3.00	1.49	1.42
24	v	615	CLA	C4B-NB	3.00	1.41	1.37
23	BB	302	CHL	CHB-C1B	3.00	1.46	1.39
25	r	615	LUT	C32-C33	-3.00	1.39	1.45
24	BQ	603	CLA	C3B-C4B	3.00	1.49	1.42
23	BJ	607	CHL	CHB-C1B	3.00	1.46	1.39
24	Au	614	CLA	C4D-ND	-3.00	1.33	1.37
25	AA	316	LUT	C8-C9	-3.00	1.39	1.45
23	0	607	CHL	CHC-C4B	3.00	1.46	1.39
24	G	614	CLA	C4D-ND	-3.00	1.33	1.37
25	6	615	LUT	C12-C13	-3.00	1.39	1.45
28	BU	616	XAT	O4-C5	-3.00	1.41	1.46
24	S	613	CLA	C4B-NB	3.00	1.41	1.37
23	AA	310	CHL	C3D-C2D	3.00	1.47	1.39
24	A6	609	CLA	C4B-NB	3.00	1.41	1.37
24	c	502	CLA	C4B-NB	3.00	1.41	1.37
24	BQ	610	CLA	C3B-C4B	3.00	1.49	1.42
29	k	101	BCR	C30-C25	-3.00	1.49	1.53
24	BE	607	CLA	C4D-ND	-3.00	1.33	1.37
28	r	616	XAT	O24-C25	-3.00	1.41	1.46
24	n	610	CLA	C3B-C4B	2.99	1.49	1.42
24	AA	305	CLA	C4B-NB	2.99	1.41	1.37
24	6	602	CLA	C3B-C4B	2.99	1.49	1.42
24	b	611	CLA	C4B-NB	2.99	1.41	1.37
25	A6	614	LUT	C8-C9	-2.99	1.39	1.45
24	C	502	CLA	C4B-NB	2.99	1.41	1.37
24	s	609	CLA	C4D-ND	-2.99	1.33	1.37
24	BJ	613	CLA	C4D-ND	-2.99	1.33	1.37
24	S	608	CLA	C4B-NB	2.99	1.41	1.37
23	n	601	CHL	C1D-C2D	2.99	1.51	1.45
25	Ba	316	LUT	C8-C9	-2.99	1.39	1.45
24	G	604	CLA	C4D-ND	-2.99	1.33	1.37
24	b	603	CLA	C4D-ND	-2.99	1.33	1.37
24	b	616	CLA	C4B-NB	2.99	1.41	1.37
24	Au	614	CLA	C4B-NB	2.99	1.41	1.37
24	BG	401	CLA	C1D-ND	2.99	1.41	1.37
23	6	607	CHL	CHB-C1B	2.99	1.46	1.39
23	6	601	CHL	C3D-C2D	2.99	1.47	1.39
23	5	606	CHL	CHB-C1B	2.99	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	310	CHL	C3D-C2D	2.99	1.47	1.39
24	A2	611	CLA	C4B-NB	2.99	1.41	1.37
23	BU	607	CHL	CHB-C1B	2.99	1.46	1.39
24	B	601	CLA	C4D-ND	-2.99	1.33	1.37
24	v	601	CLA	C4D-ND	-2.99	1.33	1.37
24	BF	502	CLA	C4B-NB	2.99	1.41	1.37
24	B	601	CLA	C3B-C4B	2.99	1.49	1.42
24	s	603	CLA	C3B-C4B	2.99	1.49	1.42
24	Y	303	CLA	C1D-ND	2.98	1.41	1.37
24	r	608	CLA	C4B-NB	2.98	1.41	1.37
24	S	608	CLA	C4D-ND	-2.98	1.33	1.37
24	BQ	602	CLA	C4D-ND	-2.98	1.33	1.37
25	N	615	LUT	C8-C9	-2.98	1.39	1.45
24	g	610	CLA	C4D-ND	-2.98	1.33	1.37
23	BU	606	CHL	CHB-C1B	2.98	1.46	1.39
28	r	616	XAT	O4-C5	-2.98	1.41	1.46
25	AA	317	LUT	C8-C9	-2.98	1.39	1.45
38	R	407	PHO	CMC-C2C	-2.98	1.45	1.50
24	y	313	CLA	C4D-ND	-2.98	1.33	1.37
24	Ba	304	CLA	C4D-ND	-2.98	1.33	1.37
25	BV	614	LUT	C8-C9	-2.98	1.39	1.45
24	a	407	CLA	C4B-NB	2.98	1.41	1.37
24	BV	611	CLA	C4B-NB	2.98	1.41	1.37
24	B	610	CLA	C4B-NB	2.98	1.41	1.37
24	Ba	313	CLA	C4D-ND	-2.98	1.33	1.37
23	8	306	CHL	C3D-C2D	2.98	1.47	1.39
24	A6	602	CLA	C4D-ND	-2.98	1.33	1.37
24	9	604	CLA	C4B-NB	2.98	1.41	1.37
24	Au	612	CLA	C4B-NB	2.98	1.41	1.37
24	BQ	612	CLA	C4D-ND	-2.97	1.33	1.37
24	7	303	CLA	C1D-ND	2.97	1.41	1.37
25	A2	616	LUT	C8-C9	-2.97	1.39	1.45
32	l	102	SQD	O47-C7	2.97	1.42	1.34
24	N	611	CLA	C4B-NB	2.97	1.41	1.37
23	BV	606	CHL	C3D-C2D	2.97	1.47	1.39
33	F	102	HEM	CAB-C3B	2.97	1.55	1.47
25	S	614	LUT	C8-C9	-2.97	1.39	1.45
24	B	605	CLA	C4B-NB	2.97	1.41	1.37
24	AA	312	CLA	C4B-NB	2.97	1.41	1.37
24	7	313	CLA	C3B-C4B	2.97	1.49	1.42
38	BD	409	PHO	CMC-C2C	-2.97	1.45	1.50
24	BG	402	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	604	CLA	C4D-ND	-2.97	1.33	1.37
23	BU	605	CHL	C1B-NB	-2.97	1.34	1.37
24	BV	604	CLA	C4D-ND	-2.97	1.33	1.37
24	G	604	CLA	C4B-NB	2.97	1.41	1.37
23	Y	307	CHL	CHB-C1B	2.97	1.46	1.39
24	g	612	CLA	C4D-ND	-2.97	1.33	1.37
25	BB	316	LUT	C8-C9	-2.97	1.39	1.45
24	Ba	312	CLA	C4B-NB	2.97	1.41	1.37
23	BB	307	CHL	CHB-C1B	2.97	1.46	1.39
24	5	604	CLA	C4B-NB	2.96	1.41	1.37
24	BJ	614	CLA	C4D-ND	-2.96	1.33	1.37
23	s	606	CHL	C3D-C2D	2.96	1.47	1.39
23	Au	605	CHL	C3D-C2D	2.96	1.47	1.39
24	n	603	CLA	C3B-C4B	2.96	1.49	1.42
24	BF	502	CLA	C3B-C4B	2.96	1.49	1.42
23	9	601	CHL	CHB-C1B	2.96	1.46	1.39
24	BE	604	CLA	C4D-ND	-2.96	1.33	1.37
24	y	312	CLA	C4B-NB	2.96	1.41	1.37
24	1	502	CLA	C3B-C4B	2.96	1.49	1.42
24	BJ	610	CLA	C4D-ND	-2.96	1.33	1.37
23	Ba	310	CHL	C1D-C2D	2.96	1.51	1.45
24	BQ	604	CLA	C4D-ND	-2.95	1.33	1.37
24	v	614	CLA	C4B-NB	2.95	1.41	1.37
24	5	603	CLA	C4B-NB	2.95	1.41	1.37
23	r	607	CHL	CHB-C1B	2.95	1.46	1.39
25	Y	316	LUT	C8-C9	-2.95	1.39	1.45
23	0	606	CHL	CHB-C1B	2.95	1.46	1.39
23	BB	306	CHL	C1B-NB	-2.95	1.34	1.37
24	BV	602	CLA	C3B-C4B	2.95	1.49	1.42
24	BU	612	CLA	C1D-ND	2.95	1.41	1.37
23	5	601	CHL	CHB-C1B	2.95	1.46	1.39
23	6	606	CHL	CHB-C1B	2.95	1.46	1.39
23	Ba	309	CHL	C3D-C2D	2.95	1.47	1.39
23	BJ	605	CHL	C1D-C2D	2.95	1.51	1.45
32	d	406	SQD	C24-C23	2.95	1.59	1.50
32	L	101	SQD	O47-C7	2.95	1.42	1.34
23	S	601	CHL	C3D-C2D	2.95	1.47	1.39
25	6	615	LUT	C10-C9	2.95	1.39	1.35
23	5	607	CHL	CHB-C1B	2.95	1.46	1.39
24	6	613	CLA	C4B-NB	2.95	1.41	1.37
32	BG	406	SQD	C24-C23	2.94	1.59	1.50
23	BQ	601	CHL	C1D-C2D	2.94	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C4B-NB	2.94	1.41	1.37
24	BE	616	CLA	C4B-NB	2.94	1.41	1.37
23	G	605	CHL	C3D-C2D	2.94	1.47	1.39
24	v	601	CLA	C3B-C4B	2.94	1.49	1.42
25	g	615	LUT	C8-C9	-2.94	1.39	1.45
24	s	612	CLA	C4D-ND	-2.94	1.33	1.37
24	s	609	CLA	C3B-C4B	2.94	1.49	1.42
23	n	607	CHL	C1D-C2D	2.94	1.51	1.45
24	s	604	CLA	C4D-ND	-2.94	1.33	1.37
25	N	616	LUT	C8-C9	-2.94	1.39	1.45
24	BJ	603	CLA	C3B-C4B	2.94	1.49	1.42
23	BJ	609	CHL	C3B-C4B	2.94	1.49	1.42
23	9	606	CHL	C1D-C2D	2.94	1.51	1.45
23	BQ	609	CHL	C3B-C4B	2.94	1.49	1.42
32	l	102	SQD	C24-C23	2.94	1.59	1.50
24	Aw	102	CLA	C1D-ND	2.94	1.41	1.37
29	B	623	BCR	C30-C25	-2.94	1.49	1.53
23	9	609	CHL	C1C-NC	-2.94	1.33	1.37
32	BO	102	SQD	O47-C7	2.94	1.42	1.34
24	B	603	CLA	C4D-ND	-2.94	1.33	1.37
24	9	604	CLA	MG-NB	-2.94	2.00	2.05
24	7	305	CLA	C3B-C4B	2.94	1.49	1.42
24	s	602	CLA	C3B-C4B	2.93	1.49	1.42
24	d	401	CLA	C1D-ND	2.93	1.41	1.37
23	BJ	601	CHL	C1D-C2D	2.93	1.51	1.45
23	AB	306	CHL	C3D-C2D	2.93	1.47	1.39
24	S	602	CLA	C4D-ND	-2.93	1.33	1.37
24	Y	313	CLA	C4B-NB	2.93	1.41	1.37
31	d	403	PL9	C36-C34	-2.93	1.45	1.51
23	BJ	608	CHL	C3D-C2D	2.93	1.47	1.39
23	n	609	CHL	C1D-C2D	2.93	1.51	1.45
24	8	303	CLA	C1D-ND	2.93	1.41	1.37
24	A2	613	CLA	C4B-NB	2.93	1.41	1.37
24	BV	613	CLA	C4B-NB	2.93	1.41	1.37
24	BF	505	CLA	C4B-NB	2.93	1.41	1.37
24	b	602	CLA	C3B-C4B	2.93	1.49	1.42
24	Y	305	CLA	C4B-NB	2.93	1.41	1.37
23	y	302	CHL	C1D-C2D	2.93	1.51	1.45
23	G	609	CHL	C3B-C4B	2.93	1.49	1.42
23	g	609	CHL	C3B-C4B	2.93	1.49	1.42
24	C	511	CLA	MG-NB	-2.93	2.00	2.05
24	9	610	CLA	C3B-C4B	2.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	305	CLA	C3B-C4B	2.93	1.49	1.42
23	Ba	310	CHL	MG-NA	-2.93	1.99	2.06
24	BU	614	CLA	C4D-ND	-2.93	1.33	1.37
24	N	613	CLA	C4B-NB	2.92	1.41	1.37
24	BB	315	CLA	C4B-NB	2.92	1.41	1.37
24	BD	405	CLA	C4B-NB	2.92	1.41	1.37
24	BE	615	CLA	C4B-NB	2.92	1.41	1.37
23	y	310	CHL	MG-NA	-2.92	1.99	2.06
24	s	602	CLA	C4D-ND	-2.92	1.33	1.37
32	BO	102	SQD	C24-C23	2.92	1.59	1.50
24	0	610	CLA	C3B-C4B	2.92	1.49	1.42
24	B	612	CLA	C1D-ND	2.92	1.41	1.37
25	7	317	LUT	C8-C9	-2.92	1.39	1.45
23	g	606	CHL	C3D-C2D	2.92	1.47	1.39
24	7	314	CLA	C4B-NB	2.92	1.41	1.37
24	8	303	CLA	C4B-NB	2.92	1.41	1.37
23	Ba	310	CHL	C3B-C4B	2.92	1.49	1.42
24	B	614	CLA	C4B-NB	2.92	1.41	1.37
24	n	613	CLA	C4D-ND	-2.92	1.33	1.37
23	BQ	609	CHL	C1D-C2D	2.92	1.51	1.45
25	S	615	LUT	C8-C9	-2.92	1.39	1.45
24	BJ	610	CLA	C3B-C4B	2.92	1.49	1.42
24	Y	312	CLA	C4B-NB	2.92	1.41	1.37
24	v	611	CLA	C4B-NB	2.92	1.41	1.37
24	g	610	CLA	C3B-C4B	2.92	1.49	1.42
38	a	409	PHO	CMC-C2C	-2.92	1.45	1.50
23	g	605	CHL	C1D-C2D	2.91	1.51	1.45
23	5	605	CHL	C1D-C2D	2.91	1.51	1.45
23	Au	605	CHL	C1D-C2D	2.91	1.51	1.45
23	g	608	CHL	C3D-C2D	2.91	1.47	1.39
24	BV	603	CLA	C3B-C4B	2.91	1.49	1.42
23	BH	601	CHL	C3D-C2D	2.91	1.47	1.39
33	4	102	HEM	CAB-C3B	2.91	1.55	1.47
24	g	604	CLA	C3B-C4B	2.91	1.49	1.42
24	BJ	604	CLA	C3B-C4B	2.91	1.49	1.42
23	e	601	CHL	C3D-C2D	2.91	1.47	1.39
24	a	405	CLA	C4B-NB	2.91	1.41	1.37
24	A6	612	CLA	C4B-NB	2.91	1.41	1.37
32	Az	101	SQD	O47-C7	2.91	1.42	1.34
24	I	102	CLA	C1D-ND	2.91	1.41	1.37
24	c	504	CLA	C4B-NB	2.91	1.41	1.37
24	AB	303	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	307	CHL	C1D-C2D	2.91	1.51	1.45
23	5	609	CHL	C3D-C2D	2.91	1.47	1.39
23	BJ	606	CHL	C3D-C2D	2.91	1.47	1.39
24	s	610	CLA	C3B-C4B	2.91	1.49	1.42
25	BB	317	LUT	C8-C9	-2.91	1.39	1.45
24	r	609	CLA	C1D-ND	2.91	1.41	1.37
28	Ba	301	XAT	O4-C5	-2.91	1.42	1.46
23	0	607	CHL	CHB-C1B	2.91	1.45	1.39
23	A6	607	CHL	C3D-C2D	2.91	1.47	1.39
24	v	610	CLA	C4B-NB	2.91	1.41	1.37
23	g	607	CHL	C1D-C2D	2.91	1.51	1.45
24	A6	613	CLA	C4B-NB	2.91	1.41	1.37
23	BQ	608	CHL	C3D-C2D	2.91	1.47	1.39
24	b	608	CLA	C4B-NB	2.90	1.41	1.37
23	A6	601	CHL	C3D-C2D	2.90	1.47	1.39
23	BV	607	CHL	C1D-C2D	2.90	1.51	1.45
24	s	613	CLA	C4B-NB	2.90	1.41	1.37
24	Au	604	CLA	C4B-NB	2.90	1.41	1.37
24	1	502	CLA	C4B-NB	2.90	1.41	1.37
24	n	602	CLA	C4D-ND	-2.90	1.33	1.37
32	D	406	SQD	C24-C23	2.90	1.59	1.50
24	v	605	CLA	C4B-NB	2.90	1.41	1.37
23	n	607	CHL	C3D-C2D	2.90	1.47	1.39
32	a	412	SQD	C24-C23	2.90	1.59	1.50
24	BV	612	CLA	C4D-ND	-2.90	1.33	1.37
24	g	611	CLA	C3B-C4B	2.90	1.49	1.42
24	c	512	CLA	C4B-NB	2.90	1.41	1.37
24	AA	314	CLA	C4B-NB	2.90	1.41	1.37
24	BD	407	CLA	C4B-NB	2.90	1.41	1.37
23	Ba	302	CHL	C3D-C2D	2.90	1.47	1.39
24	5	603	CLA	C3B-C4B	2.90	1.49	1.42
23	BQ	606	CHL	C3D-C2D	2.90	1.47	1.39
24	Ba	312	CLA	C3B-C4B	2.90	1.49	1.42
23	y	310	CHL	C1D-C2D	2.90	1.51	1.45
23	9	607	CHL	C1B-NB	-2.90	1.34	1.37
23	BB	310	CHL	C1B-NB	-2.90	1.34	1.37
24	g	603	CLA	C3B-C4B	2.90	1.49	1.42
23	6	605	CHL	C3D-C2D	2.90	1.47	1.39
24	BB	304	CLA	C4B-NB	2.90	1.41	1.37
24	S	602	CLA	C4B-NB	2.90	1.41	1.37
25	r	615	LUT	C28-C29	-2.90	1.39	1.45
23	BU	605	CHL	CHC-C1C	2.90	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	609	CHL	MG-NA	-2.89	1.99	2.06
24	A6	610	CLA	C3B-C4B	2.89	1.49	1.42
24	BV	609	CLA	C3B-C4B	2.89	1.49	1.42
23	BJ	607	CHL	C1D-C2D	2.89	1.51	1.45
25	Y	317	LUT	C8-C9	-2.89	1.39	1.45
23	g	605	CHL	C3D-C2D	2.89	1.47	1.39
24	5	612	CLA	C4B-NB	2.89	1.41	1.37
24	B	608	CLA	C4B-NB	2.89	1.41	1.37
24	AB	303	CLA	C4B-NB	2.89	1.41	1.37
24	5	614	CLA	C4D-ND	-2.89	1.33	1.37
24	s	610	CLA	C4D-ND	-2.89	1.33	1.37
23	BJ	609	CHL	MG-NA	-2.89	1.99	2.06
24	S	610	CLA	C3B-C4B	2.89	1.49	1.42
24	BV	610	CLA	C3B-C4B	2.89	1.49	1.42
23	g	601	CHL	C3D-C2D	2.89	1.47	1.39
23	BJ	601	CHL	C3D-C2D	2.89	1.47	1.39
24	g	611	CLA	C4D-ND	-2.89	1.33	1.37
23	Ba	307	CHL	C3D-C2D	2.89	1.47	1.39
24	BU	609	CLA	C1D-ND	2.89	1.41	1.37
23	y	307	CHL	C3D-C2D	2.89	1.47	1.39
32	l	101	SQD	C24-C23	2.89	1.59	1.50
24	BV	609	CLA	C4B-NB	2.89	1.41	1.37
24	BJ	611	CLA	C3B-C4B	2.89	1.49	1.42
24	y	312	CLA	C3B-C4B	2.89	1.49	1.42
32	BD	412	SQD	C24-C23	2.89	1.59	1.50
23	g	607	CHL	C3D-C2D	2.89	1.47	1.39
23	5	606	CHL	C1D-C2D	2.89	1.51	1.45
23	y	306	CHL	C3D-C2D	2.89	1.47	1.39
24	9	614	CLA	C4D-ND	-2.88	1.33	1.37
23	S	606	CHL	C3D-C2D	2.88	1.47	1.39
24	B	602	CLA	C4B-NB	2.88	1.41	1.37
28	y	301	XAT	O4-C5	-2.88	1.42	1.46
23	BQ	607	CHL	C3D-C2D	2.88	1.47	1.39
24	B	611	CLA	C4B-NB	2.88	1.41	1.37
23	Ba	302	CHL	C1D-C2D	2.88	1.51	1.45
32	BO	101	SQD	C24-C23	2.88	1.59	1.50
23	9	605	CHL	C1D-C2D	2.88	1.51	1.45
24	g	613	CLA	C3B-C4B	2.88	1.49	1.42
23	g	601	CHL	C1D-C2D	2.88	1.51	1.45
23	y	302	CHL	C3D-C2D	2.88	1.47	1.39
24	BQ	613	CLA	C1B-C2B	2.88	1.50	1.43
33	4	102	HEM	FE-ND	2.88	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	613	CLA	C1B-C2B	2.88	1.50	1.43
32	A	413	SQD	C24-C23	2.88	1.59	1.50
25	BJ	615	LUT	C8-C9	-2.88	1.39	1.45
23	9	605	CHL	C3D-C2D	2.88	1.47	1.39
32	Az	101	SQD	C24-C23	2.88	1.59	1.50
23	s	607	CHL	C1D-C2D	2.88	1.51	1.45
24	C	503	CLA	C4B-NB	2.88	1.41	1.37
23	A2	609	CHL	C1B-NB	-2.88	1.34	1.37
24	G	613	CLA	C4B-NB	2.88	1.41	1.37
23	N	609	CHL	C1B-NB	-2.87	1.34	1.37
23	BJ	605	CHL	C3D-C2D	2.87	1.47	1.39
24	BE	602	CLA	C3B-C4B	2.87	1.49	1.42
28	9	619	XAT	O4-C5	-2.87	1.42	1.46
23	A2	607	CHL	C1B-NB	-2.87	1.34	1.37
24	c	506	CLA	C4B-NB	2.87	1.41	1.37
24	BJ	611	CLA	C4D-ND	-2.87	1.33	1.37
23	5	609	CHL	C1C-NC	-2.87	1.33	1.37
24	AA	304	CLA	C3B-C4B	2.87	1.49	1.42
23	9	607	CHL	CHB-C1B	2.87	1.45	1.39
23	g	609	CHL	MG-NA	-2.87	1.99	2.06
24	N	610	CLA	C3B-C4B	2.87	1.49	1.42
23	0	607	CHL	C1B-NB	-2.87	1.34	1.37
24	n	602	CLA	C3B-C4B	2.87	1.49	1.42
23	6	609	CHL	C3D-C2D	2.87	1.46	1.39
23	n	608	CHL	C3D-C2D	2.87	1.46	1.39
23	BQ	607	CHL	C1D-C2D	2.87	1.51	1.45
23	Ba	309	CHL	C1D-C2D	2.87	1.51	1.45
23	8	306	CHL	MG-NA	-2.87	1.99	2.06
33	F	102	HEM	FE-ND	2.87	2.03	1.94
23	BJ	607	CHL	C3D-C2D	2.87	1.46	1.39
23	BJ	608	CHL	C1D-C2D	2.87	1.51	1.45
23	7	308	CHL	CHB-C1B	2.87	1.45	1.39
23	Ba	306	CHL	C3D-C2D	2.87	1.46	1.39
24	BQ	602	CLA	C3B-C4B	2.87	1.49	1.42
23	A6	606	CHL	C3D-C2D	2.86	1.46	1.39
24	v	603	CLA	C4D-ND	-2.86	1.33	1.37
24	BF	506	CLA	C4B-NB	2.86	1.41	1.37
24	7	304	CLA	C3B-C4B	2.86	1.49	1.42
23	n	609	CHL	C3B-C4B	2.86	1.49	1.42
24	v	602	CLA	C4B-NB	2.86	1.41	1.37
23	AA	308	CHL	CHB-C1B	2.86	1.45	1.39
23	r	605	CHL	C1B-NB	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	614	CLA	C3B-C4B	2.86	1.49	1.42
24	r	614	CLA	C4D-ND	-2.86	1.33	1.37
24	BQ	613	CLA	C4D-ND	-2.86	1.33	1.37
23	0	605	CHL	C3D-C2D	2.86	1.46	1.39
25	BU	615	LUT	C28-C29	-2.86	1.39	1.45
23	5	605	CHL	C3D-C2D	2.86	1.46	1.39
23	r	606	CHL	C3D-C2D	2.86	1.46	1.39
24	BE	612	CLA	C4B-NB	2.86	1.41	1.37
24	v	608	CLA	C4B-NB	2.86	1.41	1.37
32	L	101	SQD	C24-C23	2.86	1.59	1.50
24	BB	303	CLA	C3B-C4B	2.86	1.49	1.42
23	AB	306	CHL	C1B-NB	-2.86	1.34	1.37
23	BB	306	CHL	C4B-NB	-2.86	1.34	1.37
24	BJ	602	CLA	C3B-C4B	2.85	1.49	1.42
24	BJ	613	CLA	C3B-C4B	2.85	1.49	1.42
24	5	604	CLA	MG-NB	-2.85	2.00	2.05
23	G	609	CHL	C1D-C2D	2.85	1.51	1.45
24	BJ	614	CLA	C3B-C4B	2.85	1.49	1.42
25	AB	311	LUT	C28-C29	-2.85	1.39	1.45
32	R	411	SQD	C24-C23	2.85	1.59	1.50
24	c	503	CLA	C4B-NB	2.85	1.41	1.37
25	s	615	LUT	C8-C9	-2.85	1.39	1.45
25	BV	615	LUT	C8-C9	-2.85	1.39	1.45
24	BJ	603	CLA	C4D-ND	-2.85	1.33	1.37
23	G	605	CHL	C1D-C2D	2.85	1.51	1.45
24	0	603	CLA	C4B-NB	2.85	1.41	1.37
23	0	609	CHL	C1C-NC	-2.85	1.33	1.37
24	g	614	CLA	C3B-C4B	2.85	1.49	1.42
24	9	610	CLA	C4B-NB	2.85	1.41	1.37
23	AB	306	CHL	MG-NA	-2.85	1.99	2.06
23	y	310	CHL	C3B-C4B	2.85	1.49	1.42
24	A2	610	CLA	C3B-C4B	2.85	1.49	1.42
24	BE	608	CLA	C4B-NB	2.85	1.41	1.37
24	b	617	CLA	C4B-NB	2.85	1.41	1.37
24	BB	305	CLA	C4B-NB	2.85	1.41	1.37
23	y	309	CHL	C1D-C2D	2.85	1.50	1.45
23	G	609	CHL	C4B-NB	-2.85	1.34	1.37
24	BU	603	CLA	C4B-NB	2.85	1.41	1.37
24	6	602	CLA	MG-NB	-2.85	2.00	2.05
24	BE	604	CLA	C4B-NB	2.85	1.41	1.37
23	n	609	CHL	C3D-C2D	2.84	1.46	1.39
24	BQ	614	CLA	C4D-ND	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	610	CLA	C1D-ND	2.84	1.41	1.37
23	7	310	CHL	C1D-C2D	2.84	1.50	1.45
24	9	602	CLA	C3B-C4B	2.84	1.49	1.42
38	BD	408	PHO	CMC-C2C	-2.84	1.46	1.50
24	BF	514	CLA	C3B-C4B	2.84	1.49	1.42
23	AA	310	CHL	C1D-C2D	2.84	1.50	1.45
31	2	404	PL9	C53-C6	-2.84	1.44	1.50
24	5	614	CLA	C3B-C4B	2.84	1.49	1.42
24	c	514	CLA	C3B-C4B	2.84	1.49	1.42
24	BQ	611	CLA	C3B-C4B	2.84	1.49	1.42
24	n	611	CLA	C3B-C4B	2.84	1.49	1.42
24	0	614	CLA	C4B-NB	2.84	1.41	1.37
24	5	612	CLA	C3B-C4B	2.84	1.49	1.42
24	N	603	CLA	C4B-NB	2.84	1.41	1.37
24	A	405	CLA	C4B-NB	2.84	1.41	1.37
23	A6	607	CHL	C4C-C3C	2.84	1.49	1.45
23	A6	605	CHL	C3D-C2D	2.84	1.46	1.39
24	5	613	CLA	C4B-NB	2.84	1.41	1.37
24	n	612	CLA	C3B-C4B	2.84	1.49	1.42
24	BE	617	CLA	C4B-NB	2.83	1.41	1.37
24	Y	303	CLA	C3B-C4B	2.83	1.49	1.42
24	B	603	CLA	C4B-NB	2.83	1.41	1.37
24	BE	609	CLA	C1B-C2B	2.83	1.49	1.43
24	9	603	CLA	C4B-NB	2.83	1.41	1.37
23	S	605	CHL	C3D-C2D	2.83	1.46	1.39
23	BQ	609	CHL	C3D-C2D	2.83	1.46	1.39
24	0	602	CLA	MG-NB	-2.83	2.00	2.05
23	Y	306	CHL	C1B-NB	-2.83	1.34	1.37
24	Au	611	CLA	C4B-NB	2.83	1.41	1.37
24	R	406	CLA	C4B-NB	2.83	1.41	1.37
32	A1	101	SQD	C24-C23	2.83	1.59	1.50
23	y	308	CHL	C1D-C2D	2.83	1.50	1.45
24	b	604	CLA	C4B-NB	2.83	1.41	1.37
24	8	301	CLA	C4B-NB	2.83	1.41	1.37
23	y	308	CHL	C3D-C2D	2.83	1.46	1.39
24	y	303	CLA	C3B-C4B	2.83	1.49	1.42
24	R	405	CLA	C4B-NB	2.82	1.41	1.37
23	BJ	606	CHL	C1D-C2D	2.82	1.50	1.45
24	BQ	612	CLA	C3B-C4B	2.82	1.49	1.42
23	5	607	CHL	C1B-NB	-2.82	1.34	1.37
24	6	603	CLA	C4B-NB	2.82	1.41	1.37
24	A	407	CLA	C4B-NB	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	607	CHL	C3D-C2D	2.82	1.46	1.39
24	g	602	CLA	C3B-C4B	2.82	1.49	1.42
23	g	608	CHL	C1D-C2D	2.82	1.50	1.45
23	y	306	CHL	C1D-C2D	2.82	1.50	1.45
24	A2	611	CLA	C3B-C4B	2.82	1.49	1.42
38	a	408	PHO	CMC-C2C	-2.82	1.46	1.50
24	b	612	CLA	C4B-NB	2.82	1.41	1.37
23	8	306	CHL	C1B-NB	-2.82	1.34	1.37
28	N	619	XAT	O4-C5	-2.82	1.42	1.46
23	Ba	308	CHL	C3D-C2D	2.82	1.46	1.39
24	BV	611	CLA	C3B-C4B	2.82	1.49	1.42
23	6	607	CHL	C3D-C2D	2.82	1.46	1.39
23	5	609	CHL	C3B-C4B	2.82	1.49	1.42
24	N	611	CLA	C3B-C4B	2.82	1.49	1.42
24	s	611	CLA	C3B-C4B	2.82	1.49	1.42
24	Au	611	CLA	C3B-C4B	2.82	1.49	1.42
24	S	603	CLA	C3B-C4B	2.82	1.49	1.42
23	n	606	CHL	C3D-C2D	2.82	1.46	1.39
23	BU	606	CHL	C3D-C2D	2.82	1.46	1.39
24	BQ	613	CLA	C3B-C4B	2.82	1.49	1.42
23	A6	607	CHL	C1D-C2D	2.82	1.50	1.45
24	S	602	CLA	C3B-C4B	2.82	1.49	1.42
24	R	404	CLA	C4B-NB	2.82	1.41	1.37
24	7	315	CLA	C3B-C4B	2.82	1.49	1.42
24	v	609	CLA	C4B-NB	2.82	1.41	1.37
28	A2	619	XAT	O24-C25	-2.82	1.42	1.46
23	AB	305	CHL	C3D-C2D	2.82	1.46	1.39
27	0	617	LHG	O7-C5	-2.82	1.39	1.46
24	b	613	CLA	C4B-NB	2.82	1.41	1.37
24	5	611	CLA	C3B-C4B	2.81	1.49	1.42
24	A	406	CLA	C4B-NB	2.81	1.41	1.37
24	v	616	CLA	C4B-NB	2.81	1.41	1.37
24	r	602	CLA	C1D-ND	2.81	1.41	1.37
24	8	301	CLA	C3B-C4B	2.81	1.49	1.42
24	G	611	CLA	C4B-NB	2.81	1.41	1.37
24	N	610	CLA	C4B-NB	2.81	1.41	1.37
32	L	103	SQD	C24-C23	2.81	1.58	1.50
28	g	619	XAT	O4-C5	-2.81	1.42	1.46
24	Ba	303	CLA	C3B-C4B	2.81	1.49	1.42
23	0	607	CHL	C3D-C2D	2.81	1.46	1.39
24	9	603	CLA	C3B-C4B	2.81	1.49	1.42
24	g	604	CLA	C4D-ND	-2.81	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C4B-NB	2.81	1.41	1.37
24	6	614	CLA	C4B-NB	2.81	1.41	1.37
24	C	513	CLA	C4B-NB	2.81	1.41	1.37
28	BQ	619	XAT	O4-C5	-2.81	1.42	1.46
23	G	607	CHL	C3D-C2D	2.81	1.46	1.39
25	BQ	615	LUT	C8-C9	-2.81	1.39	1.45
23	6	607	CHL	C1B-NB	-2.81	1.34	1.37
23	Y	310	CHL	C1B-NB	-2.81	1.34	1.37
24	g	603	CLA	C4D-ND	-2.81	1.33	1.37
23	g	606	CHL	C1D-C2D	2.81	1.50	1.45
23	Ba	308	CHL	C1D-C2D	2.81	1.50	1.45
23	n	605	CHL	C3D-C2D	2.81	1.46	1.39
24	8	309	CLA	C3B-C4B	2.81	1.49	1.42
24	A6	603	CLA	C3B-C4B	2.81	1.49	1.42
24	B	607	CLA	C4B-NB	2.81	1.41	1.37
24	Au	613	CLA	C4B-NB	2.81	1.41	1.37
38	R	407	PHO	CAC-C3C	-2.81	1.46	1.51
28	N	619	XAT	O24-C25	-2.81	1.42	1.46
28	G	619	XAT	O4-C5	-2.80	1.42	1.46
24	G	611	CLA	C3B-C4B	2.80	1.49	1.42
23	AB	307	CHL	C1B-NB	-2.80	1.34	1.37
23	AB	304	CHL	C3D-C2D	2.80	1.46	1.39
23	8	304	CHL	C3D-C2D	2.80	1.46	1.39
23	Y	302	CHL	C3D-C2D	2.80	1.46	1.39
24	1	503	CLA	C4B-NB	2.80	1.41	1.37
23	0	601	CHL	C1D-ND	-2.80	1.34	1.37
24	BB	312	CLA	C4B-NB	2.80	1.41	1.37
23	5	607	CHL	C3D-C2D	2.80	1.46	1.39
24	Y	314	CLA	C4B-NB	2.80	1.41	1.37
25	Ba	317	LUT	C8-C9	-2.80	1.39	1.45
24	n	614	CLA	C4D-ND	-2.80	1.33	1.37
24	C	512	CLA	C4B-NB	2.80	1.41	1.37
23	Au	607	CHL	C3D-C2D	2.80	1.46	1.39
24	AA	315	CLA	C3B-C4B	2.80	1.49	1.42
23	Y	302	CHL	C1D-C2D	2.80	1.50	1.45
23	5	601	CHL	C1D-C2D	2.80	1.50	1.45
24	C	509	CLA	C4B-NB	2.80	1.41	1.37
28	A2	619	XAT	O4-C5	-2.80	1.42	1.46
24	BJ	604	CLA	C4D-ND	-2.80	1.33	1.37
23	N	601	CHL	C1D-C2D	2.80	1.50	1.45
38	BD	408	PHO	C3B-C2B	-2.80	1.36	1.40
25	G	615	LUT	C8-C9	-2.80	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CLA	C3B-C4B	2.80	1.49	1.42
23	9	608	CHL	MG-NA	-2.80	1.99	2.06
24	9	612	CLA	C4B-NB	2.79	1.41	1.37
24	BV	603	CLA	C4D-ND	-2.79	1.33	1.37
23	7	309	CHL	C1D-C2D	2.79	1.50	1.45
23	8	305	CHL	C3D-C2D	2.79	1.46	1.39
24	AB	309	CLA	C3B-C4B	2.79	1.49	1.42
24	AB	301	CLA	C4B-NB	2.79	1.41	1.37
24	Y	313	CLA	C3B-C4B	2.79	1.49	1.42
24	8	310	CLA	C3B-C4B	2.79	1.49	1.42
24	b	609	CLA	C4B-NB	2.79	1.41	1.37
24	n	610	CLA	C4B-NB	2.79	1.41	1.37
23	r	613	CHL	C1D-C2D	2.79	1.50	1.45
24	Au	602	CLA	C4B-NB	2.79	1.41	1.37
24	s	608	CLA	C3B-C4B	2.79	1.49	1.42
24	G	612	CLA	C3B-C4B	2.79	1.49	1.42
23	6	609	CHL	C3B-C4B	2.79	1.49	1.42
23	BQ	605	CHL	C3D-C2D	2.79	1.46	1.39
24	BB	313	CLA	C4B-NB	2.79	1.41	1.37
24	b	605	CLA	C4B-NB	2.79	1.41	1.37
23	7	307	CHL	C3D-C2D	2.79	1.46	1.39
24	g	613	CLA	C1B-C2B	2.79	1.49	1.43
23	N	607	CHL	C1B-NB	-2.79	1.34	1.37
28	y	301	XAT	O24-C25	-2.79	1.42	1.46
24	A2	602	CLA	C4B-NB	2.79	1.41	1.37
25	n	615	LUT	C8-C9	-2.79	1.40	1.45
38	R	408	PHO	CMC-C2C	-2.79	1.46	1.50
24	5	602	CLA	C3B-C4B	2.78	1.49	1.42
23	0	608	CHL	C1B-NB	-2.78	1.34	1.37
24	C	513	CLA	C3B-C4B	2.78	1.49	1.42
24	0	613	CLA	C4B-NB	2.78	1.41	1.37
24	BE	611	CLA	C3B-C4B	2.78	1.49	1.42
25	0	616	LUT	C8-C9	-2.78	1.40	1.45
24	AA	303	CLA	C1D-ND	2.78	1.41	1.37
23	AA	309	CHL	C1D-C2D	2.78	1.50	1.45
24	BF	512	CLA	C4B-NB	2.78	1.41	1.37
24	1	513	CLA	C3B-C4B	2.78	1.49	1.42
23	A6	607	CHL	MG-NA	-2.78	1.99	2.06
24	6	614	CLA	C3B-C4B	2.78	1.49	1.42
28	Au	619	XAT	O4-C5	-2.78	1.42	1.46
23	0	609	CHL	C3D-C2D	2.78	1.46	1.39
27	BG	404	LHG	O7-C5	-2.78	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	602	CLA	C3B-C4B	2.78	1.49	1.42
28	5	619	XAT	O4-C5	-2.78	1.42	1.46
28	AA	318	XAT	O24-C25	-2.78	1.42	1.46
24	r	611	CLA	C3B-C4B	2.78	1.49	1.42
25	Au	615	LUT	C8-C9	-2.78	1.40	1.45
24	C	506	CLA	C4B-NB	2.78	1.41	1.37
32	2	408	SQD	C24-C23	2.78	1.58	1.50
24	9	611	CLA	C3B-C4B	2.78	1.49	1.42
25	y	317	LUT	C8-C9	-2.78	1.40	1.45
24	BE	605	CLA	C4B-NB	2.78	1.41	1.37
38	A	408	PHO	CAC-C3C	-2.78	1.46	1.51
24	B	610	CLA	C3B-C4B	2.78	1.49	1.42
25	G	616	LUT	C8-C9	-2.77	1.40	1.45
28	Y	301	XAT	O4-C5	-2.77	1.42	1.46
38	R	407	PHO	C3B-C2B	-2.77	1.36	1.40
24	C	510	CLA	C4B-NB	2.77	1.41	1.37
23	8	307	CHL	C1D-C2D	2.77	1.50	1.45
24	6	610	CLA	C1D-ND	2.77	1.41	1.37
23	s	601	CHL	C3B-C4B	2.77	1.49	1.42
28	BB	301	XAT	O4-C5	-2.77	1.42	1.46
24	n	613	CLA	C3B-C4B	2.77	1.49	1.42
24	B	616	CLA	C4B-NB	2.77	1.41	1.37
23	Au	609	CHL	C3D-C2D	2.77	1.46	1.39
23	A2	608	CHL	C1B-NB	-2.77	1.34	1.37
24	b	612	CLA	C3B-C4B	2.77	1.49	1.42
24	y	305	CLA	C3B-C4B	2.77	1.49	1.42
25	9	616	LUT	C8-C9	-2.77	1.40	1.45
23	BV	601	CHL	C3B-C4B	2.77	1.49	1.42
24	Au	602	CLA	C3B-C4B	2.77	1.49	1.42
23	AA	307	CHL	C3D-C2D	2.77	1.46	1.39
24	G	603	CLA	C4B-NB	2.77	1.41	1.37
23	n	608	CHL	C1D-C2D	2.77	1.50	1.45
24	N	612	CLA	C3B-C4B	2.77	1.49	1.42
28	Ba	301	XAT	O24-C25	-2.77	1.42	1.46
23	G	606	CHL	C3D-C2D	2.77	1.46	1.39
24	7	312	CLA	C3B-C4B	2.77	1.49	1.42
24	N	612	CLA	C4B-NB	2.76	1.41	1.37
24	BV	608	CLA	C3B-C4B	2.76	1.49	1.42
23	A6	605	CHL	C1D-C2D	2.76	1.50	1.45
24	N	604	CLA	C4B-NB	2.76	1.41	1.37
23	y	309	CHL	C3D-C2D	2.76	1.46	1.39
24	Au	604	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	613	CLA	C4B-NB	2.76	1.41	1.37
28	Au	619	XAT	O24-C25	-2.76	1.42	1.46
23	9	601	CHL	C1D-C2D	2.76	1.50	1.45
23	G	608	CHL	C3D-C2D	2.76	1.46	1.39
28	n	619	XAT	O4-C5	-2.76	1.42	1.46
28	BJ	619	XAT	O24-C25	-2.76	1.42	1.46
24	BE	612	CLA	C3B-C4B	2.76	1.49	1.42
23	Ba	306	CHL	C1D-C2D	2.76	1.50	1.45
24	8	308	CLA	C1D-ND	2.76	1.41	1.37
24	C	505	CLA	C4B-NB	2.76	1.41	1.37
24	2	403	CLA	C3B-C4B	2.76	1.49	1.42
28	7	318	XAT	O24-C25	-2.76	1.42	1.46
23	G	607	CHL	C1D-C2D	2.76	1.50	1.45
24	9	612	CLA	C3B-C4B	2.76	1.49	1.42
24	b	614	CLA	C4B-NB	2.76	1.41	1.37
23	S	606	CHL	C1D-C2D	2.76	1.50	1.45
24	B	609	CLA	C4B-NB	2.76	1.41	1.37
24	b	617	CLA	C3B-C4B	2.76	1.49	1.42
23	5	608	CHL	MG-NA	-2.76	1.99	2.06
28	7	318	XAT	O4-C5	-2.76	1.42	1.46
23	0	601	CHL	C1D-C2D	2.76	1.50	1.45
24	6	611	CLA	C4B-NB	2.76	1.41	1.37
24	1	504	CLA	C4B-NB	2.76	1.41	1.37
23	BB	308	CHL	C1B-NB	-2.76	1.34	1.37
24	r	603	CLA	C4B-NB	2.76	1.41	1.37
24	G	604	CLA	C3B-C4B	2.76	1.49	1.42
23	0	607	CHL	C4B-NB	-2.75	1.34	1.37
24	BB	303	CLA	C1D-ND	2.75	1.41	1.37
24	BU	611	CLA	C3B-C4B	2.75	1.49	1.42
24	v	609	CLA	C3B-C4B	2.75	1.49	1.42
23	y	307	CHL	C1D-C2D	2.75	1.50	1.45
24	a	407	CLA	C3B-C4B	2.75	1.49	1.42
24	BD	407	CLA	C3B-C4B	2.75	1.49	1.42
24	y	305	CLA	C1B-C2B	2.75	1.49	1.43
23	BU	605	CHL	MG-NA	-2.75	1.99	2.06
24	6	604	CLA	C4B-NB	2.75	1.41	1.37
24	r	611	CLA	C4B-NB	2.75	1.41	1.37
23	AA	302	CHL	C3B-C4B	2.75	1.49	1.42
24	Ba	305	CLA	C3B-C4B	2.75	1.49	1.42
28	AA	301	XAT	O4-C5	-2.75	1.42	1.46
24	2	402	CLA	C4B-NB	2.75	1.41	1.37
23	S	605	CHL	C1D-C2D	2.75	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BD	406	CLA	C4B-NB	2.75	1.41	1.37
24	b	611	CLA	C3B-C4B	2.75	1.49	1.42
24	BJ	613	CLA	C1B-C2B	2.75	1.49	1.43
23	Au	608	CHL	C3D-C2D	2.75	1.46	1.39
23	Au	607	CHL	C1D-C2D	2.75	1.50	1.45
24	s	608	CLA	C1B-C2B	2.75	1.49	1.43
23	n	606	CHL	C1D-C2D	2.75	1.50	1.45
24	Y	311	CLA	C3B-C4B	2.75	1.49	1.42
23	A6	606	CHL	C1D-C2D	2.75	1.50	1.45
23	BQ	606	CHL	C1D-C2D	2.75	1.50	1.45
24	Ba	315	CLA	C3B-C4B	2.75	1.49	1.42
24	Ba	305	CLA	C1B-C2B	2.75	1.49	1.43
24	S	604	CLA	C3B-C4B	2.75	1.49	1.42
23	5	601	CHL	C3D-C2D	2.75	1.46	1.39
25	Au	616	LUT	C8-C9	-2.75	1.40	1.45
24	v	616	CLA	C3B-C4B	2.75	1.49	1.42
24	BU	602	CLA	MG-NB	-2.75	2.00	2.05
24	A2	604	CLA	C4B-NB	2.75	1.41	1.37
23	n	605	CHL	C1D-C2D	2.75	1.50	1.45
24	B	602	CLA	C3B-C4B	2.74	1.49	1.42
24	v	611	CLA	C3B-C4B	2.74	1.49	1.42
23	6	601	CHL	C1B-NB	-2.74	1.34	1.37
24	1	513	CLA	C4B-NB	2.74	1.41	1.37
23	s	605	CHL	C3D-C2D	2.74	1.46	1.39
23	AB	306	CHL	C4B-NB	-2.74	1.34	1.37
23	S	601	CHL	C3B-C4B	2.74	1.49	1.42
24	D	402	CLA	C3B-C4B	2.74	1.49	1.42
23	9	601	CHL	C3D-C2D	2.74	1.46	1.39
23	0	606	CHL	C1B-NB	-2.74	1.34	1.37
24	v	612	CLA	C1D-ND	2.74	1.41	1.37
23	BQ	608	CHL	C1D-C2D	2.74	1.50	1.45
23	A2	601	CHL	C1D-C2D	2.74	1.50	1.45
24	9	610	CLA	C1D-ND	2.74	1.41	1.37
24	1	510	CLA	C4B-NB	2.74	1.41	1.37
24	A2	612	CLA	C4B-NB	2.74	1.41	1.37
24	s	603	CLA	C4D-ND	-2.74	1.33	1.37
28	BJ	619	XAT	O4-C5	-2.74	1.42	1.46
23	6	605	CHL	C1D-C2D	2.74	1.50	1.45
23	s	601	CHL	C1D-C2D	2.74	1.50	1.45
24	r	614	CLA	C1B-C2B	2.74	1.49	1.43
24	y	311	CLA	C3B-C4B	2.74	1.49	1.42
24	A6	602	CLA	C3B-C4B	2.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AB	312	XAT	O24-C25	-2.74	1.42	1.46
24	BJ	602	CLA	C1B-C2B	2.74	1.49	1.43
23	8	305	CHL	C1B-NB	-2.74	1.34	1.37
24	B	616	CLA	C3B-C4B	2.74	1.49	1.42
24	A2	612	CLA	C3B-C4B	2.74	1.49	1.42
23	N	601	CHL	C3D-C2D	2.74	1.46	1.39
24	Au	603	CLA	C4B-NB	2.74	1.41	1.37
24	d	401	CLA	C4B-NB	2.73	1.41	1.37
23	6	601	CHL	C1D-C2D	2.73	1.50	1.45
28	8	312	XAT	O24-C25	-2.73	1.42	1.46
24	BF	508	CLA	MG-NB	-2.73	2.00	2.05
23	0	608	CHL	C4B-NB	-2.73	1.34	1.37
23	BB	310	CHL	C4B-NB	-2.73	1.34	1.37
34	c	516	DGD	O2G-C2G	-2.73	1.39	1.46
24	BF	503	CLA	C4B-NB	2.73	1.41	1.37
24	BE	604	CLA	C3B-C4B	2.73	1.49	1.42
24	d	402	CLA	C3B-C4B	2.73	1.49	1.42
24	BV	612	CLA	C1B-C2B	2.73	1.49	1.43
24	Ba	314	CLA	C1B-C2B	2.73	1.49	1.43
28	G	619	XAT	O24-C25	-2.73	1.42	1.46
24	Y	304	CLA	C3B-C4B	2.73	1.49	1.42
24	A6	604	CLA	C3B-C4B	2.73	1.49	1.42
28	7	301	XAT	O4-C5	-2.73	1.42	1.46
24	v	607	CLA	C4B-NB	2.73	1.41	1.37
24	AA	312	CLA	C3B-C4B	2.73	1.49	1.42
25	8	311	LUT	C12-C13	-2.73	1.40	1.45
24	c	507	CLA	C4B-NB	2.73	1.41	1.37
23	S	607	CHL	C3D-C2D	2.73	1.46	1.39
24	0	614	CLA	C3B-C4B	2.73	1.49	1.42
24	AB	301	CLA	C3B-C4B	2.73	1.49	1.42
23	8	304	CHL	C1D-C2D	2.73	1.50	1.45
23	BU	613	CHL	C1D-C2D	2.73	1.50	1.45
24	b	604	CLA	C3B-C4B	2.73	1.49	1.42
24	BE	613	CLA	C4B-NB	2.73	1.41	1.37
38	A	408	PHO	C3B-C2B	-2.73	1.36	1.40
24	r	602	CLA	C3B-C4B	2.73	1.49	1.42
24	BB	304	CLA	C3B-C4B	2.73	1.49	1.42
24	A2	603	CLA	C4B-NB	2.73	1.41	1.37
24	A2	610	CLA	C4B-NB	2.73	1.41	1.37
23	7	302	CHL	C3B-C4B	2.73	1.49	1.42
24	B	611	CLA	C3B-C4B	2.73	1.49	1.42
25	6	615	LUT	C32-C33	-2.73	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BU	601	CLA	C3B-C4B	2.73	1.49	1.42
23	Y	310	CHL	C3D-C2D	2.72	1.46	1.39
23	9	608	CHL	C1D-ND	-2.72	1.34	1.37
24	r	601	CLA	C4B-NB	2.72	1.41	1.37
24	v	602	CLA	C3B-C4B	2.72	1.49	1.42
31	BG	403	PL9	C53-C6	-2.72	1.45	1.50
24	b	610	CLA	C1B-C2B	2.72	1.49	1.43
24	y	315	CLA	C3B-C4B	2.72	1.49	1.42
24	g	602	CLA	C1B-C2B	2.72	1.49	1.43
23	s	605	CHL	C1D-C2D	2.72	1.50	1.45
24	BE	617	CLA	C3B-C4B	2.72	1.49	1.42
24	A6	608	CLA	C3B-C4B	2.72	1.49	1.42
24	BB	313	CLA	C3B-C4B	2.72	1.49	1.42
24	N	602	CLA	C4B-NB	2.72	1.41	1.37
24	BF	510	CLA	C4B-NB	2.72	1.41	1.37
24	BU	610	CLA	MG-NB	-2.72	2.00	2.05
24	G	614	CLA	C3B-C4B	2.72	1.49	1.42
24	1	506	CLA	C4B-NB	2.72	1.41	1.37
23	BQ	605	CHL	C1D-C2D	2.72	1.50	1.45
24	r	609	CLA	MG-NB	-2.72	2.00	2.05
23	BB	302	CHL	C3D-C2D	2.72	1.46	1.39
24	s	612	CLA	C1B-C2B	2.72	1.49	1.43
23	6	608	CHL	C3D-C2D	2.72	1.46	1.39
28	g	619	XAT	O24-C25	-2.72	1.42	1.46
28	n	619	XAT	O24-C25	-2.72	1.42	1.46
23	5	605	CHL	MG-NA	-2.72	1.99	2.06
23	A2	601	CHL	C3D-C2D	2.72	1.46	1.39
23	BB	306	CHL	MG-NA	-2.72	1.99	2.06
25	BB	317	LUT	C32-C33	-2.72	1.40	1.45
23	BV	601	CHL	C1D-C2D	2.72	1.50	1.45
23	Au	606	CHL	C3D-C2D	2.72	1.46	1.39
23	Y	308	CHL	C1B-NB	-2.72	1.34	1.37
24	a	406	CLA	C4B-NB	2.72	1.41	1.37
23	6	606	CHL	C3D-C2D	2.71	1.46	1.39
24	y	314	CLA	C1B-C2B	2.71	1.49	1.43
28	AA	318	XAT	O4-C5	-2.71	1.42	1.46
23	BV	606	CHL	C1D-C2D	2.71	1.50	1.45
24	b	616	CLA	C3B-C4B	2.71	1.49	1.42
24	B	614	CLA	C1B-C2B	2.71	1.49	1.43
24	BV	608	CLA	C1B-C2B	2.71	1.49	1.43
23	6	606	CHL	C1B-NB	-2.71	1.34	1.37
23	G	609	CHL	MG-NA	-2.71	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	311	LUT	C32-C33	-2.71	1.40	1.45
23	BV	605	CHL	C3D-C2D	2.71	1.46	1.39
24	D	401	CLA	C4B-NB	2.71	1.41	1.37
24	c	514	CLA	C4B-NB	2.71	1.41	1.37
24	BJ	604	CLA	C1B-C2B	2.71	1.49	1.43
24	7	314	CLA	C1B-C2B	2.71	1.49	1.43
24	BF	510	CLA	MG-NB	-2.71	2.00	2.05
23	8	306	CHL	C4B-NB	-2.71	1.34	1.37
24	BG	402	CLA	C3B-C4B	2.71	1.49	1.42
23	0	608	CHL	C3D-C2D	2.71	1.46	1.39
24	BQ	612	CLA	C1B-C2B	2.71	1.49	1.43
28	7	301	XAT	O24-C25	-2.71	1.42	1.46
24	BU	609	CLA	MG-NB	-2.71	2.00	2.05
23	7	309	CHL	C3D-C2D	2.71	1.46	1.39
24	BE	603	CLA	C3B-C4B	2.70	1.49	1.42
38	a	408	PHO	C3B-C2B	-2.70	1.36	1.40
24	AB	310	CLA	C3B-C4B	2.70	1.49	1.42
23	6	601	CHL	C1D-ND	-2.70	1.34	1.37
38	R	407	PHO	CMB-C2B	-2.70	1.46	1.51
24	0	611	CLA	C4B-NB	2.70	1.41	1.37
24	BF	511	CLA	C3B-C4B	2.70	1.49	1.42
24	r	608	CLA	C3B-C4B	2.70	1.49	1.42
24	BE	610	CLA	C3B-C4B	2.70	1.49	1.42
24	6	612	CLA	C4B-NB	2.70	1.41	1.37
24	b	603	CLA	C3B-C4B	2.70	1.49	1.42
23	8	307	CHL	C3D-C2D	2.70	1.46	1.39
23	0	608	CHL	MG-NA	-2.70	1.99	2.06
24	BU	608	CLA	C3B-C4B	2.70	1.49	1.42
24	s	602	CLA	C1B-C2B	2.70	1.49	1.43
23	AA	309	CHL	C3D-C2D	2.70	1.46	1.39
23	0	601	CHL	C1B-NB	-2.70	1.34	1.37
23	0	605	CHL	C1D-C2D	2.70	1.50	1.45
24	B	604	CLA	C4B-NB	2.70	1.41	1.37
24	1	512	CLA	C4B-NB	2.70	1.41	1.37
23	BQ	601	CHL	C3B-C4B	2.70	1.49	1.42
24	A	407	CLA	C3B-C4B	2.70	1.49	1.42
24	v	610	CLA	C3B-C4B	2.70	1.49	1.42
24	Au	614	CLA	C3B-C4B	2.70	1.49	1.42
24	1	511	CLA	C4B-NB	2.70	1.41	1.37
23	6	608	CHL	MG-NA	-2.70	1.99	2.06
25	n	616	LUT	C8-C9	-2.70	1.40	1.45
23	AB	307	CHL	C3D-C2D	2.70	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	314	CLA	C1B-C2B	2.70	1.49	1.43
23	6	608	CHL	C1D-C2D	2.70	1.50	1.45
24	B	612	CLA	C4B-NB	2.70	1.41	1.37
24	1	509	CLA	C4B-NB	2.70	1.41	1.37
23	s	606	CHL	C1D-C2D	2.70	1.50	1.45
23	9	605	CHL	MG-NA	-2.70	1.99	2.06
24	BF	507	CLA	C4B-NB	2.70	1.41	1.37
24	g	603	CLA	C1B-C2B	2.69	1.49	1.43
24	c	505	CLA	C3B-C4B	2.69	1.49	1.42
33	f	102	HEM	FE-NB	2.69	2.03	1.94
24	a	410	CLA	C4B-NB	2.69	1.41	1.37
24	BU	602	CLA	C1D-ND	2.69	1.41	1.37
23	9	609	CHL	C1B-C2B	2.69	1.49	1.43
24	n	611	CLA	C1B-C2B	2.69	1.49	1.43
24	Au	612	CLA	C3B-C4B	2.69	1.49	1.42
24	BV	604	CLA	MG-NB	-2.69	2.00	2.05
24	A6	611	CLA	C3B-C4B	2.69	1.49	1.42
24	8	308	CLA	C3B-C4B	2.69	1.49	1.42
24	v	614	CLA	C1B-C2B	2.69	1.49	1.43
24	BB	314	CLA	C4B-NB	2.69	1.41	1.37
24	BQ	611	CLA	C1B-C2B	2.69	1.49	1.43
25	6	615	LUT	C28-C29	-2.69	1.40	1.45
25	AB	311	LUT	C12-C13	-2.69	1.40	1.45
24	BF	505	CLA	C3B-C4B	2.69	1.49	1.42
24	8	303	CLA	C1B-C2B	2.69	1.49	1.43
24	b	609	CLA	C1B-C2B	2.69	1.49	1.43
33	F	102	HEM	FE-NC	2.69	2.04	1.95
24	BF	504	CLA	C4B-NB	2.69	1.41	1.37
24	BU	611	CLA	C4B-NB	2.69	1.41	1.37
24	b	610	CLA	C3B-C4B	2.69	1.49	1.42
23	Au	609	CHL	C1D-C2D	2.69	1.50	1.45
23	S	607	CHL	MG-NA	-2.69	1.99	2.06
24	AB	302	CLA	C3B-C4B	2.69	1.49	1.42
25	0	616	LUT	C12-C13	-2.69	1.40	1.45
23	r	607	CHL	C3D-C2D	2.69	1.46	1.39
23	6	607	CHL	C4B-NB	-2.69	1.34	1.37
23	A2	606	CHL	C1B-NB	-2.69	1.34	1.37
24	9	613	CLA	C1B-C2B	2.69	1.49	1.43
24	Ba	311	CLA	C3B-C4B	2.69	1.49	1.42
23	BH	601	CHL	C1D-C2D	2.69	1.50	1.45
24	6	613	CLA	MG-NB	-2.69	2.00	2.05
24	r	610	CLA	MG-NB	-2.69	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BU	614	CLA	C3B-C4B	2.69	1.49	1.42
24	BJ	603	CLA	C1B-C2B	2.69	1.49	1.43
23	n	601	CHL	C3B-C4B	2.69	1.49	1.42
23	G	608	CHL	C1D-C2D	2.68	1.50	1.45
25	8	311	LUT	C28-C29	-2.68	1.40	1.45
24	g	610	CLA	C1B-C2B	2.68	1.49	1.43
24	s	603	CLA	C1B-C2B	2.68	1.49	1.43
24	BJ	610	CLA	C1B-C2B	2.68	1.49	1.43
28	BQ	619	XAT	O24-C25	-2.68	1.42	1.46
24	1	505	CLA	C4B-NB	2.68	1.41	1.37
24	r	603	CLA	C3B-C4B	2.68	1.49	1.42
23	7	308	CHL	C3D-C2D	2.68	1.46	1.39
23	0	609	CHL	C3B-C4B	2.68	1.49	1.42
23	8	307	CHL	C1B-NB	-2.68	1.34	1.37
23	N	608	CHL	C1B-NB	-2.68	1.34	1.37
23	A2	609	CHL	C4B-NB	-2.68	1.34	1.37
24	BQ	604	CLA	C3B-C4B	2.68	1.49	1.42
23	A6	601	CHL	C3B-C4B	2.68	1.49	1.42
38	A	409	PHO	CMC-C2C	-2.68	1.46	1.50
24	Y	312	CLA	C3B-C4B	2.68	1.49	1.42
24	r	602	CLA	MG-NB	-2.68	2.00	2.05
24	B	613	CLA	C3B-C4B	2.68	1.49	1.42
23	0	606	CHL	C3D-C2D	2.68	1.46	1.39
38	BD	408	PHO	CMD-C2D	-2.68	1.46	1.51
23	Y	306	CHL	MG-NA	-2.68	1.99	2.06
23	AB	305	CHL	C1D-C2D	2.68	1.50	1.45
23	r	605	CHL	MG-NA	-2.68	1.99	2.06
24	BE	616	CLA	C3B-C4B	2.68	1.49	1.42
23	BB	306	CHL	C3D-C2D	2.68	1.46	1.39
24	BU	611	CLA	MG-NB	-2.68	2.00	2.05
24	8	302	CLA	C3B-C4B	2.68	1.49	1.42
24	b	606	CLA	C3B-C4B	2.68	1.49	1.42
38	a	409	PHO	CMD-C2D	-2.68	1.46	1.51
23	Y	306	CHL	C3D-C2D	2.68	1.46	1.39
24	g	604	CLA	C1B-C2B	2.68	1.49	1.43
23	AB	304	CHL	C1D-C2D	2.68	1.50	1.45
23	AA	308	CHL	C3D-C2D	2.67	1.46	1.39
24	0	612	CLA	C3B-C4B	2.67	1.49	1.42
33	4	102	HEM	FE-NC	2.67	2.04	1.95
24	B	609	CLA	C3B-C4B	2.67	1.49	1.42
23	Au	608	CHL	C1D-C2D	2.67	1.50	1.45
24	6	612	CLA	C3B-C4B	2.67	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BE	610	CLA	C1B-C2B	2.67	1.49	1.43
24	BB	311	CLA	C3B-C4B	2.67	1.49	1.42
24	BV	602	CLA	C1B-C2B	2.67	1.49	1.43
23	AB	305	CHL	C1B-NB	-2.67	1.34	1.37
23	6	609	CHL	C1D-C2D	2.67	1.50	1.45
24	n	612	CLA	C1B-C2B	2.67	1.49	1.43
24	v	612	CLA	C4B-NB	2.67	1.41	1.37
24	BU	601	CLA	C4B-NB	2.67	1.41	1.37
33	BI	102	HEM	FE-NA	2.67	2.04	1.95
23	N	606	CHL	C1B-NB	-2.67	1.34	1.37
24	G	610	CLA	C3B-C4B	2.67	1.49	1.42
27	BB	319	LHG	O7-C5	-2.67	1.39	1.46
23	Y	306	CHL	C4B-NB	-2.67	1.34	1.37
25	6	616	LUT	C8-C9	-2.67	1.40	1.45
24	c	510	CLA	C4B-NB	2.67	1.41	1.37
23	BJ	601	CHL	C3B-C4B	2.67	1.49	1.42
38	A	408	PHO	CMB-C2B	-2.67	1.46	1.51
24	c	511	CLA	C3B-C4B	2.67	1.49	1.42
28	AA	301	XAT	O24-C25	-2.67	1.42	1.46
23	N	608	CHL	C3D-C2D	2.67	1.46	1.39
24	R	406	CLA	C3B-C4B	2.67	1.49	1.42
23	5	608	CHL	C1D-ND	-2.67	1.34	1.37
23	AA	310	CHL	C1D-ND	-2.67	1.34	1.37
24	8	309	CLA	C1B-C2B	2.67	1.49	1.43
24	AB	309	CLA	C1B-C2B	2.67	1.49	1.43
23	A6	607	CHL	C1D-ND	-2.67	1.34	1.37
24	c	513	CLA	C4B-NB	2.67	1.41	1.37
24	BG	401	CLA	C4B-NB	2.67	1.41	1.37
27	6	617	LHG	O7-C5	-2.67	1.39	1.46
24	0	613	CLA	MG-NB	-2.67	2.00	2.05
24	A2	613	CLA	C1B-C2B	2.67	1.49	1.43
24	r	601	CLA	C3B-C4B	2.66	1.49	1.42
24	n	602	CLA	C1B-C2B	2.66	1.49	1.43
24	b	615	CLA	C3B-C4B	2.66	1.49	1.42
24	C	510	CLA	C3B-C4B	2.66	1.49	1.42
24	S	611	CLA	C3B-C4B	2.66	1.49	1.42
24	BE	606	CLA	C3B-C4B	2.66	1.49	1.42
23	A2	608	CHL	C3D-C2D	2.66	1.46	1.39
24	AB	301	CLA	C1B-C2B	2.66	1.49	1.43
24	BQ	602	CLA	C1B-C2B	2.66	1.49	1.43
23	Y	310	CHL	C4B-NB	-2.66	1.34	1.37
23	9	608	CHL	C4B-NB	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C3B-C4B	2.66	1.49	1.42
24	8	308	CLA	MG-NB	-2.66	2.00	2.05
24	AB	308	CLA	MG-NB	-2.66	2.00	2.05
24	BU	602	CLA	C3B-C4B	2.66	1.49	1.42
24	BF	511	CLA	MG-NB	-2.66	2.00	2.05
24	N	603	CLA	C3B-C4B	2.66	1.49	1.42
24	BU	614	CLA	C1B-C2B	2.66	1.49	1.43
24	S	611	CLA	C4B-NB	2.66	1.41	1.37
23	5	605	CHL	C4B-NB	-2.66	1.34	1.37
24	r	610	CLA	C4B-NB	2.66	1.41	1.37
23	BB	302	CHL	C1D-C2D	2.66	1.50	1.45
24	d	401	CLA	C3B-C4B	2.66	1.49	1.42
24	n	604	CLA	C3B-C4B	2.66	1.49	1.42
24	v	613	CLA	C3B-C4B	2.66	1.49	1.42
23	AB	307	CHL	MG-NA	-2.66	2.00	2.06
23	AB	306	CHL	C1D-ND	-2.66	1.34	1.37
24	c	510	CLA	MG-NB	-2.65	2.00	2.05
24	S	612	CLA	C1B-C2B	2.65	1.49	1.43
23	6	608	CHL	C1B-NB	-2.65	1.34	1.37
24	A6	613	CLA	C3B-C4B	2.65	1.49	1.42
24	BV	612	CLA	C3B-C4B	2.65	1.49	1.42
24	v	603	CLA	C4B-NB	2.65	1.41	1.37
24	g	611	CLA	C1B-C2B	2.65	1.49	1.43
23	g	601	CHL	C3B-C4B	2.65	1.49	1.42
23	BB	307	CHL	C1B-NB	-2.65	1.34	1.37
23	s	605	CHL	C3B-C4B	2.65	1.49	1.42
24	n	604	CLA	C1B-C2B	2.65	1.49	1.43
24	s	612	CLA	C3B-C4B	2.65	1.49	1.42
24	8	302	CLA	C1B-C2B	2.65	1.49	1.43
24	y	314	CLA	C3B-C4B	2.65	1.49	1.42
24	Ba	314	CLA	C3B-C4B	2.65	1.49	1.42
24	r	614	CLA	C3B-C4B	2.65	1.49	1.42
24	BU	601	CLA	MG-NB	-2.65	2.00	2.05
24	v	605	CLA	C1B-C2B	2.65	1.49	1.43
23	0	607	CHL	C1D-C2D	2.65	1.50	1.45
23	6	607	CHL	MG-NA	-2.65	2.00	2.06
24	C	511	CLA	C3B-C4B	2.65	1.49	1.42
24	C	511	CLA	C4B-NB	2.65	1.41	1.37
24	Au	613	CLA	C1B-C2B	2.65	1.49	1.43
23	BU	607	CHL	C3D-C2D	2.65	1.46	1.39
24	G	613	CLA	C1B-C2B	2.65	1.49	1.43
23	Y	310	CHL	C1D-C2D	2.65	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BD	409	PHO	CMD-C2D	-2.64	1.46	1.51
24	5	613	CLA	C1B-C2B	2.64	1.49	1.43
23	N	605	CHL	C3D-C2D	2.64	1.46	1.39
24	BD	410	CLA	C4B-NB	2.64	1.41	1.37
25	BU	615	LUT	C12-C13	-2.64	1.40	1.45
24	BJ	614	CLA	C1B-C2B	2.64	1.49	1.43
23	n	607	CHL	C3B-C4B	2.64	1.49	1.42
24	BB	312	CLA	C3B-C4B	2.64	1.49	1.42
23	5	601	CHL	C4C-C3C	2.64	1.49	1.45
38	R	408	PHO	CMD-C2D	-2.64	1.46	1.51
24	BV	603	CLA	C1B-C2B	2.64	1.49	1.43
25	BB	316	LUT	C32-C33	-2.64	1.40	1.45
24	BU	610	CLA	C4B-NB	2.64	1.41	1.37
25	9	615	LUT	C8-C9	-2.64	1.40	1.45
23	y	302	CHL	C3B-C4B	2.64	1.48	1.42
23	G	601	CHL	C3D-C2D	2.64	1.46	1.39
24	B	612	CLA	MG-NB	-2.64	2.00	2.05
24	I	102	CLA	MG-NB	-2.64	2.00	2.05
23	Y	307	CHL	C1B-NB	-2.64	1.34	1.37
24	5	602	CLA	C4B-NB	2.64	1.41	1.37
23	0	605	CHL	MG-NA	-2.64	2.00	2.06
25	Y	317	LUT	C32-C33	-2.64	1.40	1.45
25	r	615	LUT	C12-C13	-2.64	1.40	1.45
24	B	603	CLA	C3B-C4B	2.64	1.48	1.42
24	A	410	CLA	C3B-C4B	2.64	1.48	1.42
38	BD	409	PHO	CAC-C3C	-2.64	1.46	1.51
24	b	615	CLA	C1B-C2B	2.64	1.49	1.43
24	BU	603	CLA	C3B-C4B	2.64	1.48	1.42
23	Au	609	CHL	C1B-NB	-2.64	1.34	1.37
24	r	609	CLA	C4B-NB	2.64	1.41	1.37
24	0	614	CLA	MG-NB	-2.64	2.00	2.05
23	Ba	307	CHL	C1D-C2D	2.64	1.50	1.45
23	N	607	CHL	C3D-C2D	2.64	1.46	1.39
23	5	607	CHL	C1D-ND	-2.64	1.34	1.37
23	6	609	CHL	C1D-ND	-2.64	1.34	1.37
23	Ba	302	CHL	C3B-C4B	2.64	1.48	1.42
24	C	508	CLA	C4B-NB	2.64	1.41	1.37
24	BV	609	CLA	C1B-C2B	2.64	1.49	1.43
24	v	604	CLA	C4B-NB	2.64	1.41	1.37
23	BV	607	CHL	C3B-C4B	2.64	1.48	1.42
24	5	610	CLA	C4B-NB	2.64	1.41	1.37
24	BJ	611	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BV	611	CLA	C1B-C2B	2.64	1.49	1.43
31	2	404	PL9	C52-C5	-2.64	1.45	1.50
23	0	607	CHL	MG-NA	-2.63	2.00	2.06
24	n	610	CLA	C1B-C2B	2.63	1.49	1.43
24	BF	514	CLA	C4B-NB	2.63	1.41	1.37
23	5	608	CHL	C3D-C2D	2.63	1.46	1.39
23	N	606	CHL	C3D-C2D	2.63	1.46	1.39
24	c	511	CLA	MG-NB	-2.63	2.00	2.05
24	9	603	CLA	MG-NB	-2.63	2.00	2.05
24	N	613	CLA	C1B-C2B	2.63	1.49	1.43
33	F	102	HEM	FE-NB	2.63	2.03	1.94
23	6	607	CHL	C1D-C2D	2.63	1.50	1.45
24	AB	303	CLA	C1B-C2B	2.63	1.49	1.43
25	AA	317	LUT	C32-C33	-2.63	1.40	1.45
24	C	505	CLA	C3B-C4B	2.63	1.48	1.42
24	Au	610	CLA	C3B-C4B	2.63	1.48	1.42
24	r	612	CLA	C4B-NB	2.63	1.41	1.37
23	e	601	CHL	C1D-C2D	2.63	1.50	1.45
23	8	305	CHL	C1D-C2D	2.63	1.50	1.45
24	b	613	CLA	C1B-C2B	2.63	1.49	1.43
24	b	602	CLA	C1B-C2B	2.63	1.49	1.43
23	s	607	CHL	C3B-C4B	2.63	1.48	1.42
24	v	605	CLA	C3B-C4B	2.63	1.48	1.42
24	BB	305	CLA	C3B-C4B	2.63	1.48	1.42
24	B	613	CLA	C4B-NB	2.63	1.41	1.37
24	g	614	CLA	C1B-C2B	2.63	1.49	1.43
24	v	612	CLA	MG-NB	-2.63	2.00	2.05
24	A2	602	CLA	C3B-C4B	2.63	1.48	1.42
24	BV	613	CLA	C3B-C4B	2.63	1.48	1.42
24	BE	602	CLA	C1B-C2B	2.63	1.49	1.43
23	BB	310	CHL	C3D-C2D	2.63	1.46	1.39
27	d	404	LHG	O7-C5	-2.63	1.40	1.46
23	8	306	CHL	C1D-ND	-2.63	1.34	1.37
23	9	606	CHL	C1B-NB	-2.63	1.34	1.37
23	N	607	CHL	C1D-C2D	2.63	1.50	1.45
23	6	605	CHL	MG-NA	-2.63	2.00	2.06
24	B	607	CLA	C3B-C4B	2.62	1.48	1.42
23	BU	605	CHL	C4B-NB	-2.62	1.34	1.37
24	A6	602	CLA	C4B-NB	2.62	1.41	1.37
23	0	608	CHL	C1D-C2D	2.62	1.50	1.45
23	BV	605	CHL	C1D-C2D	2.62	1.50	1.45
24	7	303	CLA	CMC-C2C	-2.62	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	606	CHL	C1D-C2D	2.62	1.50	1.45
24	b	606	CLA	C1B-C2B	2.62	1.49	1.43
24	AB	302	CLA	C1B-C2B	2.62	1.49	1.43
28	Y	301	XAT	O24-C25	-2.62	1.42	1.46
23	8	304	CHL	MG-NA	-2.62	2.00	2.06
24	A2	603	CLA	C3B-C4B	2.62	1.48	1.42
24	S	603	CLA	C1B-C2B	2.62	1.49	1.43
24	Ba	304	CLA	C1B-C2B	2.62	1.49	1.43
24	S	613	CLA	C3B-C4B	2.62	1.48	1.42
38	R	407	PHO	CMD-C2D	-2.62	1.46	1.51
24	v	615	CLA	C3B-C4B	2.62	1.48	1.42
24	B	601	CLA	C1B-C2B	2.62	1.49	1.43
23	7	310	CHL	C1D-ND	-2.62	1.34	1.37
23	BQ	607	CHL	C3B-C4B	2.62	1.48	1.42
24	BE	615	CLA	C3B-C4B	2.62	1.48	1.42
23	A2	606	CHL	C3D-C2D	2.62	1.46	1.39
24	0	604	CLA	C4B-NB	2.62	1.41	1.37
24	BU	603	CLA	MG-NB	-2.62	2.00	2.05
23	G	609	CHL	C4C-C3C	2.62	1.49	1.45
23	BV	605	CHL	C3B-C4B	2.62	1.48	1.42
24	d	402	CLA	C1B-C2B	2.62	1.49	1.43
23	6	608	CHL	C4B-NB	-2.62	1.34	1.37
23	A2	607	CHL	C3D-C2D	2.62	1.46	1.39
24	6	604	CLA	C1B-C2B	2.62	1.49	1.43
23	9	605	CHL	C4B-NB	-2.62	1.34	1.37
23	r	613	CHL	C3D-C2D	2.61	1.46	1.39
24	BE	606	CLA	C1B-C2B	2.61	1.49	1.43
24	r	603	CLA	MG-NB	-2.61	2.00	2.05
24	1	510	CLA	C3B-C4B	2.61	1.48	1.42
24	Y	305	CLA	C3B-C4B	2.61	1.48	1.42
33	BI	102	HEM	FE-NB	2.61	2.02	1.94
24	v	601	CLA	C1B-C2B	2.61	1.49	1.43
24	b	614	CLA	C3B-C4B	2.61	1.48	1.42
24	B	605	CLA	C1B-C2B	2.61	1.49	1.43
24	v	612	CLA	CMD-C2D	-2.61	1.45	1.50
24	BE	616	CLA	C1B-C2B	2.61	1.49	1.43
24	0	612	CLA	C4B-NB	2.61	1.41	1.37
24	B	605	CLA	C3B-C4B	2.61	1.48	1.42
24	BF	509	CLA	C3B-C4B	2.61	1.48	1.42
24	BF	507	CLA	CMB-C2B	-2.61	1.45	1.50
23	9	608	CHL	C3D-C2D	2.61	1.46	1.39
23	9	601	CHL	C3B-C4B	2.61	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	609	CLA	C1B-C2B	2.61	1.49	1.43
25	AA	316	LUT	C32-C33	-2.61	1.40	1.45
24	A	405	CLA	C3B-C4B	2.61	1.48	1.42
24	v	603	CLA	C3B-C4B	2.61	1.48	1.42
24	b	611	CLA	C3C-C2C	2.61	1.42	1.36
23	s	607	CHL	C4C-C3C	2.61	1.49	1.45
24	1	505	CLA	C3B-C4B	2.61	1.48	1.42
24	BE	614	CLA	C4B-NB	2.61	1.41	1.37
23	5	609	CHL	C1B-C2B	2.61	1.49	1.43
24	c	505	CLA	C1B-C2B	2.61	1.49	1.43
24	s	611	CLA	C1B-C2B	2.61	1.49	1.43
31	d	403	PL9	C53-C6	-2.61	1.45	1.50
23	A2	607	CHL	C1D-C2D	2.61	1.50	1.45
24	c	506	CLA	C3B-C4B	2.61	1.48	1.42
24	r	601	CLA	MG-NB	-2.60	2.00	2.05
25	5	615	LUT	C8-C9	-2.60	1.40	1.45
24	R	409	CLA	C3B-C4B	2.60	1.48	1.42
24	Ba	303	CLA	C1B-C2B	2.60	1.49	1.43
23	g	609	CHL	C4C-C3C	2.60	1.49	1.45
23	9	601	CHL	C4C-C3C	2.60	1.49	1.45
24	AA	311	CLA	C3B-C4B	2.60	1.48	1.42
24	AB	308	CLA	CMC-C2C	-2.60	1.45	1.50
23	Ba	307	CHL	C1B-C2B	2.60	1.49	1.43
23	N	609	CHL	C4B-NB	-2.60	1.34	1.37
23	BU	606	CHL	MG-NA	-2.60	2.00	2.06
24	s	613	CLA	C3B-C4B	2.60	1.48	1.42
24	c	509	CLA	C4B-NB	2.60	1.41	1.37
24	A6	611	CLA	C4B-NB	2.60	1.41	1.37
24	c	509	CLA	C3B-C4B	2.60	1.48	1.42
28	BB	301	XAT	O24-C25	-2.60	1.42	1.46
24	R	404	CLA	C3B-C4B	2.60	1.48	1.42
24	r	611	CLA	MG-NB	-2.60	2.00	2.05
23	g	609	CHL	C1B-NB	-2.60	1.34	1.37
23	5	609	CHL	C4C-C3C	2.60	1.49	1.45
23	7	308	CHL	C1D-C2D	2.60	1.50	1.45
23	9	606	CHL	C3D-C2D	2.60	1.46	1.39
24	n	603	CLA	C1B-C2B	2.60	1.49	1.43
24	0	610	CLA	C4B-NB	2.60	1.41	1.37
38	a	409	PHO	CAC-C3C	-2.60	1.46	1.51
23	6	601	CHL	C3B-C4B	2.60	1.48	1.42
23	Au	601	CHL	C1B-NB	-2.60	1.34	1.37
24	G	610	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	612	CLA	C1B-C2B	2.60	1.49	1.43
25	7	317	LUT	C32-C33	-2.60	1.40	1.45
24	AA	314	CLA	C3B-C4B	2.60	1.48	1.42
23	5	608	CHL	C4B-NB	-2.60	1.34	1.37
24	5	611	CLA	C1B-C2B	2.60	1.49	1.43
23	G	606	CHL	C1D-C2D	2.60	1.50	1.45
23	y	307	CHL	C1B-C2B	2.59	1.49	1.43
24	D	401	CLA	C3B-C4B	2.59	1.48	1.42
23	S	607	CHL	C1D-C2D	2.59	1.50	1.45
24	A6	612	CLA	C1B-C2B	2.59	1.49	1.43
24	9	602	CLA	C4B-NB	2.59	1.41	1.37
24	B	608	CLA	C3B-C4B	2.59	1.48	1.42
24	A	405	CLA	C1B-C2B	2.59	1.49	1.43
23	AB	307	CHL	C4B-NB	-2.59	1.34	1.37
34	BF	518	DGD	O2G-C2G	-2.59	1.40	1.46
24	N	602	CLA	C3B-C4B	2.59	1.48	1.42
24	BB	313	CLA	MG-NB	-2.59	2.00	2.05
24	0	612	CLA	C1B-C2B	2.59	1.49	1.43
24	AB	303	CLA	C3B-C4B	2.59	1.48	1.42
24	8	301	CLA	C1B-C2B	2.59	1.49	1.43
23	G	608	CHL	MG-NA	-2.59	2.00	2.06
23	Y	309	CHL	C3B-C4B	2.59	1.48	1.42
24	y	303	CLA	C1B-C2B	2.59	1.49	1.43
24	c	512	CLA	C3B-C4B	2.59	1.48	1.42
24	BU	609	CLA	C4B-NB	2.59	1.41	1.37
23	BB	308	CHL	C3D-C2D	2.59	1.46	1.39
24	6	614	CLA	MG-NB	-2.59	2.00	2.05
24	BU	609	CLA	CMC-C2C	-2.59	1.45	1.50
23	Au	601	CHL	C3D-C2D	2.59	1.46	1.39
38	BD	408	PHO	CMB-C2B	-2.59	1.46	1.51
24	7	304	CLA	C1B-C2B	2.59	1.49	1.43
24	y	304	CLA	C1B-C2B	2.59	1.49	1.43
24	9	611	CLA	C1B-C2B	2.59	1.49	1.43
24	BE	615	CLA	C1B-C2B	2.59	1.49	1.43
23	Au	608	CHL	MG-NA	-2.59	2.00	2.06
24	7	314	CLA	C3B-C4B	2.59	1.48	1.42
23	A2	605	CHL	C3D-C2D	2.59	1.46	1.39
38	R	408	PHO	CMB-C2B	-2.59	1.46	1.51
33	f	102	HEM	FE-NA	2.59	2.03	1.95
24	5	603	CLA	MG-NB	-2.59	2.00	2.05
24	BF	513	CLA	C4B-NB	2.59	1.41	1.37
24	S	604	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	304	CHL	MG-NA	-2.59	2.00	2.06
25	y	316	LUT	C32-C33	-2.59	1.40	1.45
24	g	612	CLA	C1B-C2B	2.59	1.49	1.43
24	BJ	612	CLA	C1B-C2B	2.59	1.49	1.43
24	Ba	313	CLA	C1B-C2B	2.59	1.49	1.43
23	BQ	608	CHL	C3B-C4B	2.59	1.48	1.42
24	C	512	CLA	C3B-C4B	2.59	1.48	1.42
23	r	606	CHL	MG-NA	-2.58	2.00	2.06
24	6	612	CLA	C1B-C2B	2.58	1.49	1.43
23	y	310	CHL	C4C-C3C	2.58	1.49	1.45
23	BJ	609	CHL	C4C-C3C	2.58	1.49	1.45
23	A2	608	CHL	C1D-ND	-2.58	1.34	1.37
23	BU	606	CHL	C1D-C2D	2.58	1.50	1.45
23	BU	606	CHL	C4B-NB	-2.58	1.34	1.37
23	BB	309	CHL	C3B-C4B	2.58	1.48	1.42
23	n	608	CHL	C1B-C2B	2.58	1.49	1.43
23	5	601	CHL	C3B-C4B	2.58	1.48	1.42
23	Au	606	CHL	C1D-C2D	2.58	1.50	1.45
24	Aw	102	CLA	MG-NB	-2.58	2.00	2.05
24	Au	614	CLA	C1B-C2B	2.58	1.49	1.43
23	0	601	CHL	C3B-C4B	2.58	1.48	1.42
23	BB	310	CHL	C1D-ND	-2.58	1.34	1.37
24	G	602	CLA	C4B-NB	2.58	1.41	1.37
24	BF	509	CLA	C4B-NB	2.58	1.41	1.37
24	Ba	315	CLA	C1B-C2B	2.58	1.49	1.43
24	B	614	CLA	C3B-C4B	2.58	1.48	1.42
24	Y	315	CLA	C3B-C4B	2.58	1.48	1.42
23	N	605	CHL	C1B-C2B	2.58	1.49	1.43
23	Y	308	CHL	C3D-C2D	2.58	1.46	1.39
24	7	313	CLA	C1B-C2B	2.58	1.49	1.43
23	0	609	CHL	C1D-C2D	2.58	1.50	1.45
23	5	606	CHL	C1B-NB	-2.58	1.34	1.37
23	BJ	609	CHL	C1B-NB	-2.58	1.34	1.37
24	y	315	CLA	C1B-C2B	2.58	1.49	1.43
24	b	608	CLA	C3B-C4B	2.58	1.48	1.42
24	BU	608	CLA	C1B-C2B	2.58	1.49	1.43
24	AA	304	CLA	C1B-C2B	2.58	1.49	1.43
24	R	404	CLA	C1B-C2B	2.58	1.49	1.43
24	BE	614	CLA	C3B-C4B	2.58	1.48	1.42
23	BJ	605	CHL	C1B-C2B	2.58	1.49	1.43
38	a	408	PHO	CMD-C2D	-2.58	1.46	1.51
24	b	616	CLA	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	604	CLA	MG-NB	-2.57	2.00	2.05
24	BF	503	CLA	MG-NB	-2.57	2.00	2.05
23	Au	607	CHL	C3B-C4B	2.57	1.48	1.42
23	9	609	CHL	C1D-C2D	2.57	1.50	1.45
24	1	509	CLA	MG-NB	-2.57	2.00	2.05
23	Y	306	CHL	C1D-C2D	2.57	1.50	1.45
23	BV	607	CHL	C1B-C2B	2.57	1.49	1.43
24	v	609	CLA	C1B-C2B	2.57	1.49	1.43
24	BF	506	CLA	CMD-C2D	-2.57	1.45	1.50
23	Ba	306	CHL	MG-NA	-2.57	2.00	2.06
33	4	102	HEM	FE-NB	2.57	2.02	1.94
23	AA	306	CHL	C1B-C2B	2.57	1.49	1.43
24	BG	402	CLA	C1B-C2B	2.57	1.49	1.43
38	A	409	PHO	CMB-C2B	-2.57	1.46	1.51
38	BD	408	PHO	CAC-C3C	-2.57	1.47	1.51
24	Y	314	CLA	C1B-C2B	2.57	1.49	1.43
24	BB	314	CLA	C1B-C2B	2.57	1.49	1.43
24	c	511	CLA	C4B-NB	2.57	1.40	1.37
23	S	601	CHL	C1D-C2D	2.57	1.50	1.45
24	8	303	CLA	C3B-C4B	2.57	1.48	1.42
34	1	517	DGD	O2G-C2G	-2.57	1.40	1.46
23	s	607	CHL	C1B-C2B	2.57	1.49	1.43
24	v	607	CLA	C3B-C4B	2.57	1.48	1.42
25	Y	316	LUT	C32-C33	-2.57	1.40	1.45
24	1	506	CLA	CMB-C2B	-2.57	1.45	1.50
25	BQ	616	LUT	C8-C9	-2.57	1.40	1.45
24	A6	603	CLA	C1B-C2B	2.57	1.49	1.43
24	BQ	603	CLA	C1B-C2B	2.57	1.49	1.43
23	g	608	CHL	C3B-C4B	2.57	1.48	1.42
24	Au	610	CLA	C4B-NB	2.57	1.40	1.37
23	6	605	CHL	C3B-C4B	2.57	1.48	1.42
38	A	408	PHO	CMD-C2D	-2.57	1.46	1.51
24	BG	401	CLA	C3B-C4B	2.57	1.48	1.42
24	r	604	CLA	MG-NB	-2.57	2.00	2.05
24	v	613	CLA	C4B-NB	2.57	1.40	1.37
24	r	604	CLA	C3B-C4B	2.57	1.48	1.42
23	BB	306	CHL	C1D-ND	-2.57	1.34	1.37
23	AA	307	CHL	C1D-C2D	2.57	1.50	1.45
24	Au	613	CLA	C3B-C4B	2.57	1.48	1.42
38	R	407	PHO	C4D-ND	-2.57	1.35	1.38
23	Ba	309	CHL	C1B-C2B	2.57	1.49	1.43
24	S	612	CLA	C3B-C4B	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	606	CHL	C3D-C2D	2.57	1.46	1.39
24	v	614	CLA	C3B-C4B	2.56	1.48	1.42
24	2	402	CLA	C3B-C4B	2.56	1.48	1.42
24	BU	604	CLA	MG-NB	-2.56	2.00	2.05
24	b	609	CLA	C3B-C4B	2.56	1.48	1.42
24	BF	506	CLA	C3B-C4B	2.56	1.48	1.42
38	a	408	PHO	CAC-C3C	-2.56	1.47	1.51
23	Y	309	CHL	C3D-C2D	2.56	1.46	1.39
38	A	409	PHO	CMD-C2D	-2.56	1.46	1.51
24	c	503	CLA	C3B-C4B	2.56	1.48	1.42
23	r	605	CHL	C4B-NB	-2.56	1.34	1.37
23	7	307	CHL	C1D-C2D	2.56	1.50	1.45
24	G	603	CLA	C3B-C4B	2.56	1.48	1.42
23	N	608	CHL	C1D-ND	-2.56	1.34	1.37
24	r	608	CLA	C1B-C2B	2.56	1.49	1.43
24	8	310	CLA	C1B-C2B	2.56	1.49	1.43
24	A	410	CLA	C4B-NB	2.56	1.40	1.37
24	C	508	CLA	MG-NB	-2.56	2.00	2.05
24	BE	613	CLA	MG-NB	-2.56	2.00	2.05
24	B	607	CLA	C1B-C2B	2.56	1.49	1.43
24	G	614	CLA	C1B-C2B	2.56	1.49	1.43
24	1	511	CLA	C1B-C2B	2.56	1.49	1.43
24	A2	604	CLA	C3B-C4B	2.56	1.48	1.42
24	v	608	CLA	C3B-C4B	2.56	1.48	1.42
24	c	503	CLA	MG-NB	-2.56	2.00	2.05
27	b	624	LHG	O7-C5	-2.56	1.40	1.46
24	D	402	CLA	C1B-C2B	2.56	1.49	1.43
24	2	403	CLA	C1B-C2B	2.56	1.49	1.43
24	c	508	CLA	MG-NB	-2.56	2.00	2.05
33	f	102	HEM	FE-ND	2.56	2.02	1.94
24	b	608	CLA	C1B-C2B	2.56	1.49	1.43
24	BE	608	CLA	C3B-C4B	2.56	1.48	1.42
27	BE	624	LHG	O7-C5	-2.56	1.40	1.46
24	6	604	CLA	MG-NB	-2.56	2.00	2.05
24	A6	604	CLA	C1B-C2B	2.56	1.49	1.43
24	6	604	CLA	C3B-C4B	2.56	1.48	1.42
38	A	408	PHO	C4D-ND	-2.56	1.35	1.38
23	y	306	CHL	MG-NA	-2.56	2.00	2.06
23	BB	310	CHL	C1D-C2D	2.56	1.50	1.45
24	N	604	CLA	C3B-C4B	2.56	1.48	1.42
24	n	614	CLA	C1B-C2B	2.56	1.49	1.43
38	R	408	PHO	CAC-C3C	-2.56	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	306	CHL	C1B-C2B	2.56	1.49	1.43
27	Az	102	LHG	O7-C5	-2.56	1.40	1.46
24	BQ	604	CLA	C1B-C2B	2.56	1.49	1.43
24	C	511	CLA	C1B-C2B	2.55	1.49	1.43
24	BU	612	CLA	MG-NB	-2.55	2.00	2.05
24	b	613	CLA	C3B-C4B	2.55	1.48	1.42
23	0	605	CHL	C3B-C4B	2.55	1.48	1.42
23	y	309	CHL	C1B-C2B	2.55	1.49	1.43
24	v	615	CLA	C1B-C2B	2.55	1.49	1.43
23	n	608	CHL	C3B-C4B	2.55	1.48	1.42
24	BU	604	CLA	C3B-C4B	2.55	1.48	1.42
24	C	507	CLA	C4B-NB	2.55	1.40	1.37
24	B	612	CLA	CMD-C2D	-2.55	1.45	1.50
23	A6	601	CHL	C1B-NB	-2.55	1.34	1.37
23	BU	613	CHL	C1B-NB	-2.55	1.34	1.37
24	8	303	CLA	MG-NB	-2.55	2.00	2.05
24	Au	612	CLA	C1B-C2B	2.55	1.49	1.43
23	AA	302	CHL	C1B-NB	-2.55	1.34	1.37
24	0	604	CLA	C1B-C2B	2.55	1.49	1.43
38	BD	409	PHO	CMB-C2B	-2.55	1.46	1.51
24	0	603	CLA	MG-NB	-2.55	2.00	2.05
23	BV	607	CHL	C4C-C3C	2.55	1.49	1.45
23	8	307	CHL	C3B-C4B	2.55	1.48	1.42
23	BH	601	CHL	C3B-C4B	2.55	1.48	1.42
34	Av	102	DGD	O1G-C1G	-2.55	1.39	1.45
23	7	306	CHL	C4C-C3C	2.55	1.49	1.45
24	r	612	CLA	MG-NB	-2.55	2.00	2.05
27	L	102	LHG	O7-C5	-2.55	1.40	1.46
23	N	608	CHL	C4B-NB	-2.55	1.34	1.37
38	a	408	PHO	CMB-C2B	-2.55	1.46	1.51
24	A6	612	CLA	C3B-C4B	2.55	1.48	1.42
24	c	507	CLA	C3B-C4B	2.55	1.48	1.42
24	Au	603	CLA	C3B-C4B	2.55	1.48	1.42
23	n	601	CHL	C1B-C2B	2.54	1.49	1.43
23	BQ	601	CHL	C1B-C2B	2.54	1.49	1.43
24	AA	303	CLA	MG-NB	-2.54	2.00	2.05
23	e	601	CHL	C3B-C4B	2.54	1.48	1.42
24	y	313	CLA	C1B-C2B	2.54	1.49	1.43
23	g	605	CHL	C1B-C2B	2.54	1.49	1.43
23	AB	304	CHL	C1B-NB	-2.54	1.34	1.37
23	BJ	608	CHL	C3B-C4B	2.54	1.48	1.42
24	9	602	CLA	MG-NB	-2.54	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	603	CLA	MG-NB	-2.54	2.00	2.05
24	BB	303	CLA	MG-NB	-2.54	2.00	2.05
24	BB	315	CLA	C3B-C4B	2.54	1.48	1.42
24	r	610	CLA	C3B-C4B	2.54	1.48	1.42
25	A2	616	LUT	C32-C33	-2.54	1.40	1.45
24	1	507	CLA	C4B-NB	2.54	1.40	1.37
24	2	402	CLA	C1B-C2B	2.54	1.49	1.43
24	AA	303	CLA	CMC-C2C	-2.54	1.45	1.50
24	AA	303	CLA	C4B-NB	2.54	1.40	1.37
25	G	615	LUT	C12-C13	-2.54	1.40	1.45
25	AA	316	LUT	C12-C13	-2.54	1.40	1.45
23	N	608	CHL	C1D-C2D	2.54	1.50	1.45
23	AA	308	CHL	C1D-C2D	2.54	1.50	1.45
23	BQ	608	CHL	C1B-C2B	2.54	1.49	1.43
24	BQ	614	CLA	C1B-C2B	2.54	1.49	1.43
24	7	303	CLA	C3B-C4B	2.54	1.48	1.42
23	y	309	CHL	C3B-C4B	2.54	1.48	1.42
24	B	609	CLA	MG-NB	-2.54	2.00	2.05
23	A2	605	CHL	C1D-C2D	2.54	1.50	1.45
23	N	608	CHL	MG-NA	-2.54	2.00	2.06
24	N	613	CLA	C3B-C4B	2.54	1.48	1.42
24	AA	303	CLA	C3B-C4B	2.54	1.48	1.42
24	0	602	CLA	C3B-C4B	2.54	1.48	1.42
23	G	601	CHL	C1D-C2D	2.54	1.50	1.45
23	N	605	CHL	C1D-C2D	2.54	1.50	1.45
25	A6	614	LUT	C12-C13	-2.54	1.40	1.45
24	c	513	CLA	C3B-C4B	2.54	1.48	1.42
23	9	607	CHL	C1D-ND	-2.54	1.34	1.37
23	0	609	CHL	C1B-C2B	2.54	1.49	1.43
24	G	612	CLA	C1B-C2B	2.54	1.49	1.43
23	BU	613	CHL	C3D-C2D	2.54	1.46	1.39
23	5	601	CHL	C1B-NB	-2.54	1.34	1.37
23	5	608	CHL	C1D-C2D	2.54	1.50	1.45
25	S	614	LUT	C12-C13	-2.54	1.40	1.45
24	C	506	CLA	C3B-C4B	2.54	1.48	1.42
24	R	409	CLA	MG-NB	-2.53	2.00	2.05
25	N	615	LUT	C32-C33	-2.53	1.40	1.45
24	a	406	CLA	C1B-C2B	2.53	1.49	1.43
24	1	512	CLA	C3B-C4B	2.53	1.48	1.42
24	BU	608	CLA	MG-NB	-2.53	2.00	2.05
24	B	615	CLA	C1B-C2B	2.53	1.49	1.43
25	5	616	LUT	C8-C9	-2.53	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BU	610	CLA	C3B-C4B	2.53	1.48	1.42
24	B	602	CLA	C1B-C2B	2.53	1.49	1.43
24	BE	613	CLA	C1B-C2B	2.53	1.49	1.43
25	7	316	LUT	C32-C33	-2.53	1.40	1.45
24	7	311	CLA	C3B-C4B	2.53	1.48	1.42
23	A6	607	CHL	C1B-NB	-2.53	1.34	1.37
24	C	505	CLA	C1B-C2B	2.53	1.49	1.43
24	BE	608	CLA	C1B-C2B	2.53	1.49	1.43
38	A	409	PHO	CAC-C3C	-2.53	1.47	1.51
23	Au	605	CHL	C1B-C2B	2.53	1.49	1.43
24	b	614	CLA	C1B-C2B	2.53	1.49	1.43
24	1	507	CLA	MG-NB	-2.53	2.00	2.05
23	r	613	CHL	C1B-NB	-2.53	1.34	1.37
23	5	609	CHL	C1D-C2D	2.53	1.50	1.45
23	A6	607	CHL	C3B-C4B	2.53	1.48	1.42
23	BB	309	CHL	C3D-C2D	2.53	1.46	1.39
23	AA	306	CHL	MG-NA	-2.53	2.00	2.06
24	0	604	CLA	MG-NB	-2.53	2.00	2.05
24	1	508	CLA	MG-NB	-2.53	2.00	2.05
24	BD	410	CLA	C3B-C4B	2.53	1.48	1.42
24	r	608	CLA	MG-NB	-2.53	2.00	2.05
23	AA	306	CHL	C4C-C3C	2.53	1.49	1.45
33	BI	102	HEM	FE-ND	2.53	2.02	1.94
24	5	614	CLA	C1B-C2B	2.53	1.49	1.43
23	5	607	CHL	C3B-C4B	2.53	1.48	1.42
24	0	611	CLA	C3B-C4B	2.53	1.48	1.42
24	y	311	CLA	C1B-C2B	2.53	1.49	1.43
24	BU	612	CLA	C1B-C2B	2.53	1.49	1.43
24	BG	401	CLA	MG-NB	-2.53	2.00	2.05
23	A2	608	CHL	MG-NA	-2.53	2.00	2.06
23	A6	601	CHL	C1D-C2D	2.53	1.50	1.45
23	5	607	CHL	C4B-NB	-2.53	1.34	1.37
23	BU	607	CHL	C1B-NB	-2.53	1.34	1.37
25	7	316	LUT	C12-C13	-2.53	1.40	1.45
23	BQ	606	CHL	C1B-C2B	2.53	1.49	1.43
24	B	612	CLA	C1B-C2B	2.53	1.49	1.43
23	BB	306	CHL	C1D-C2D	2.52	1.50	1.45
24	G	613	CLA	C3B-C4B	2.52	1.48	1.42
24	Y	314	CLA	MG-NB	-2.52	2.00	2.05
23	AA	302	CHL	MG-NA	-2.52	2.00	2.06
24	BD	405	CLA	C1B-C2B	2.52	1.49	1.43
23	N	609	CHL	C1D-C2D	2.52	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BE	604	CLA	C1B-C2B	2.52	1.49	1.43
23	Au	606	CHL	C1B-NB	-2.52	1.34	1.37
23	A2	609	CHL	C1D-ND	-2.52	1.34	1.37
24	v	612	CLA	C1B-C2B	2.52	1.49	1.43
23	8	305	CHL	C1D-ND	-2.52	1.34	1.37
24	7	303	CLA	C4B-NB	2.52	1.40	1.37
24	b	605	CLA	C1B-C2B	2.52	1.49	1.43
24	c	513	CLA	MG-NB	-2.52	2.00	2.05
23	Ba	310	CHL	C4C-C3C	2.52	1.49	1.45
24	D	401	CLA	C1B-C2B	2.52	1.49	1.43
23	A6	607	CHL	C4B-NB	-2.52	1.34	1.37
34	H	102	DGD	O1G-C1G	-2.52	1.39	1.45
23	Ba	309	CHL	MG-NA	-2.52	2.00	2.06
24	c	508	CLA	C1B-C2B	2.52	1.49	1.43
24	2	402	CLA	MG-NB	-2.52	2.00	2.05
23	n	606	CHL	C1B-C2B	2.52	1.49	1.43
23	A2	608	CHL	C4B-NB	-2.52	1.34	1.37
24	a	410	CLA	C3B-C4B	2.52	1.48	1.42
24	0	603	CLA	C3B-C4B	2.52	1.48	1.42
24	1	511	CLA	C3B-C4B	2.52	1.48	1.42
25	Au	615	LUT	C12-C13	-2.52	1.40	1.45
23	y	309	CHL	MG-NA	-2.52	2.00	2.06
34	C	517	DGD	O2G-C2G	-2.52	1.40	1.46
23	Ba	310	CHL	C1B-C2B	2.52	1.49	1.43
24	BE	603	CLA	C1B-C2B	2.52	1.49	1.43
24	A2	613	CLA	C3B-C4B	2.52	1.48	1.42
24	BF	505	CLA	C1B-C2B	2.52	1.49	1.43
24	5	602	CLA	MG-NB	-2.52	2.00	2.05
24	A	410	CLA	MG-NB	-2.52	2.00	2.05
23	r	605	CHL	CHC-C4B	2.52	1.45	1.39
23	AA	308	CHL	C1B-NB	-2.52	1.34	1.37
24	6	610	CLA	C4B-NB	2.52	1.40	1.37
23	A2	605	CHL	C1B-C2B	2.52	1.49	1.43
23	Y	307	CHL	C3D-C2D	2.52	1.46	1.39
23	y	307	CHL	C3B-C4B	2.51	1.48	1.42
23	6	605	CHL	C1B-C2B	2.51	1.49	1.43
24	6	611	CLA	C3B-C4B	2.51	1.48	1.42
23	G	605	CHL	C1B-C2B	2.51	1.49	1.43
24	BF	503	CLA	CMB-C2B	-2.51	1.45	1.50
24	b	603	CLA	C1B-C2B	2.51	1.49	1.43
38	a	409	PHO	CMB-C2B	-2.51	1.46	1.51
23	s	606	CHL	C3B-C4B	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	606	CHL	C4B-NB	-2.51	1.34	1.37
23	BU	613	CHL	C1D-ND	-2.51	1.34	1.37
24	9	613	CLA	MG-NB	-2.51	2.00	2.05
24	Y	313	CLA	MG-NB	-2.51	2.00	2.05
24	S	610	CLA	C1B-C2B	2.51	1.49	1.43
24	BV	610	CLA	C1B-C2B	2.51	1.49	1.43
23	BV	606	CHL	C3B-C4B	2.51	1.48	1.42
24	5	613	CLA	C3B-C4B	2.51	1.48	1.42
23	N	606	CHL	C1D-C2D	2.51	1.50	1.45
25	Ba	316	LUT	C32-C33	-2.51	1.40	1.45
31	BG	403	PL9	C52-C5	-2.51	1.45	1.50
24	C	513	CLA	C1B-C2B	2.51	1.49	1.43
23	9	601	CHL	C1B-NB	-2.51	1.34	1.37
24	r	604	CLA	C4B-NB	2.51	1.40	1.37
24	A2	610	CLA	MG-NB	-2.51	2.00	2.05
25	A2	615	LUT	C32-C33	-2.51	1.40	1.45
23	Au	607	CHL	C1B-C2B	2.51	1.49	1.43
29	BE	618	BCR	C30-C25	-2.51	1.50	1.53
23	Ba	306	CHL	C1B-NB	-2.51	1.34	1.37
24	1	508	CLA	C4B-NB	2.51	1.40	1.37
24	BB	311	CLA	MG-NB	-2.51	2.00	2.05
23	Ba	307	CHL	C3B-C4B	2.51	1.48	1.42
23	r	607	CHL	C1B-NB	-2.51	1.34	1.37
24	AA	315	CLA	C1B-C2B	2.51	1.49	1.43
23	AB	307	CHL	C1D-ND	-2.51	1.34	1.37
24	1	512	CLA	MG-NB	-2.51	2.00	2.05
24	c	506	CLA	CMD-C2D	-2.51	1.45	1.50
23	y	310	CHL	C1B-C2B	2.51	1.49	1.43
24	BV	613	CLA	C1B-C2B	2.51	1.49	1.43
24	7	315	CLA	C1B-C2B	2.51	1.49	1.43
24	AB	303	CLA	MG-NB	-2.51	2.00	2.05
23	7	306	CHL	MG-NA	-2.51	2.00	2.06
23	BB	307	CHL	C3D-C2D	2.51	1.46	1.39
24	a	406	CLA	C3B-C4B	2.51	1.48	1.42
24	5	610	CLA	MG-NB	-2.51	2.00	2.05
24	BQ	610	CLA	C1B-C2B	2.50	1.49	1.43
23	G	601	CHL	C1B-NB	-2.50	1.34	1.37
24	BD	406	CLA	C1B-C2B	2.50	1.49	1.43
25	6	616	LUT	C12-C13	-2.50	1.40	1.45
24	C	503	CLA	C3B-C4B	2.50	1.48	1.42
24	BF	513	CLA	MG-NB	-2.50	2.00	2.05
23	5	608	CHL	C1B-NB	-2.50	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	0	609	CHL	C1D-ND	-2.50	1.34	1.37
24	9	612	CLA	MG-NB	-2.50	2.00	2.05
24	R	409	CLA	C4B-NB	2.50	1.40	1.37
24	Y	311	CLA	C1B-C2B	2.50	1.49	1.43
24	B	604	CLA	C1B-C2B	2.50	1.49	1.43
24	A2	611	CLA	C1B-C2B	2.50	1.49	1.43
24	N	614	CLA	C1B-C2B	2.50	1.49	1.43
24	Y	311	CLA	MG-NB	-2.50	2.00	2.05
24	7	311	CLA	C1B-C2B	2.50	1.49	1.43
24	G	611	CLA	C1B-C2B	2.50	1.49	1.43
23	7	302	CHL	MG-NA	-2.50	2.00	2.06
23	g	605	CHL	C3B-C4B	2.50	1.48	1.42
24	AA	313	CLA	C1B-C2B	2.50	1.49	1.43
27	BE	623	LHG	O7-C5	-2.50	1.40	1.46
24	Y	314	CLA	C3B-C4B	2.50	1.48	1.42
23	G	606	CHL	C1B-NB	-2.50	1.34	1.37
23	Y	302	CHL	C3B-C4B	2.50	1.48	1.42
24	BB	314	CLA	MG-NB	-2.50	2.00	2.05
24	BF	508	CLA	C1B-C2B	2.50	1.49	1.43
23	s	606	CHL	C1B-C2B	2.50	1.49	1.43
24	9	614	CLA	C1B-C2B	2.50	1.49	1.43
23	Au	601	CHL	C1D-C2D	2.50	1.50	1.45
23	7	306	CHL	C3B-C4B	2.50	1.48	1.42
23	AB	307	CHL	C3B-C4B	2.50	1.48	1.42
34	BF	517	DGD	O2G-C2G	-2.50	1.40	1.46
23	A2	606	CHL	C1D-C2D	2.50	1.50	1.45
24	A2	604	CLA	C1B-C2B	2.50	1.49	1.43
24	BB	305	CLA	CMB-C2B	-2.50	1.45	1.50
26	N	617	NEX	C12-C13	-2.50	1.40	1.45
23	5	605	CHL	C1B-NB	-2.50	1.34	1.37
23	9	609	CHL	C4C-C3C	2.50	1.49	1.45
23	7	302	CHL	C1B-NB	-2.50	1.34	1.37
24	A2	614	CLA	C1B-C2B	2.50	1.49	1.43
24	C	509	CLA	MG-NB	-2.50	2.00	2.05
24	1	510	CLA	MG-NB	-2.50	2.00	2.05
24	C	506	CLA	CMB-C2B	-2.50	1.45	1.50
23	BJ	605	CHL	C3B-C4B	2.50	1.48	1.42
24	A	406	CLA	C3B-C4B	2.50	1.48	1.42
24	C	510	CLA	C1B-C2B	2.49	1.49	1.43
24	C	504	CLA	C1B-C2B	2.49	1.49	1.43
34	c	517	DGD	O2G-C2G	-2.49	1.40	1.46
24	C	503	CLA	MG-NB	-2.49	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	304	CHL	C1B-C2B	2.49	1.49	1.43
24	Y	305	CLA	C1B-C2B	2.49	1.49	1.43
23	BJ	607	CHL	C3B-C4B	2.49	1.48	1.42
24	BB	303	CLA	CMB-C2B	-2.49	1.45	1.50
24	7	303	CLA	MG-NB	-2.49	2.00	2.05
24	c	504	CLA	C3B-C4B	2.49	1.48	1.42
23	9	607	CHL	C4B-NB	-2.49	1.34	1.37
24	s	610	CLA	C1B-C2B	2.49	1.49	1.43
24	Ba	311	CLA	C1B-C2B	2.49	1.49	1.43
23	r	605	CHL	C3D-C2D	2.49	1.45	1.39
24	BF	503	CLA	C3B-C4B	2.49	1.48	1.42
23	g	608	CHL	C1B-C2B	2.49	1.49	1.43
24	A6	610	CLA	C1B-C2B	2.49	1.49	1.43
25	BB	316	LUT	C12-C13	-2.49	1.40	1.45
24	1	505	CLA	C1B-C2B	2.49	1.49	1.43
23	9	606	CHL	C4B-NB	-2.49	1.34	1.37
24	v	607	CLA	C1B-C2B	2.49	1.49	1.43
24	1	503	CLA	MG-NB	-2.49	2.00	2.05
23	7	308	CHL	C1B-NB	-2.49	1.34	1.37
23	BV	606	CHL	C1B-C2B	2.49	1.49	1.43
23	A6	605	CHL	C3B-C4B	2.49	1.48	1.42
24	v	604	CLA	MG-NB	-2.49	2.00	2.05
24	b	604	CLA	C1B-C2B	2.49	1.49	1.43
24	a	405	CLA	C1B-C2B	2.49	1.49	1.43
24	BB	315	CLA	MG-NB	-2.49	2.00	2.05
26	A2	617	NEX	C32-C33	-2.49	1.40	1.45
23	S	605	CHL	C3B-C4B	2.49	1.48	1.42
23	A2	608	CHL	C1D-C2D	2.49	1.50	1.45
24	BF	507	CLA	C3B-C4B	2.48	1.48	1.42
25	A6	614	LUT	C32-C33	-2.48	1.40	1.45
24	C	508	CLA	C3B-C4B	2.48	1.48	1.42
24	S	613	CLA	C1B-C2B	2.48	1.49	1.43
24	r	610	CLA	C1B-C2B	2.48	1.49	1.43
24	5	612	CLA	MG-NB	-2.48	2.00	2.05
23	9	609	CHL	C1D-ND	-2.48	1.34	1.37
24	N	611	CLA	C1B-C2B	2.48	1.49	1.43
24	8	308	CLA	CMD-C2D	-2.48	1.45	1.50
24	BU	602	CLA	CMC-C2C	-2.48	1.45	1.50
25	Au	616	LUT	C28-C29	-2.48	1.40	1.45
23	g	607	CHL	C3B-C4B	2.48	1.48	1.42
23	8	306	CHL	C1D-C2D	2.48	1.50	1.45
24	AB	308	CLA	CHC-C1C	2.48	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	302	CLA	MG-NB	-2.48	2.00	2.05
23	Ba	309	CHL	C3B-C4B	2.48	1.48	1.42
24	N	604	CLA	C1B-C2B	2.48	1.49	1.43
27	2	405	LHG	O7-C5	-2.48	1.40	1.46
38	BD	408	PHO	C4D-ND	-2.48	1.35	1.38
23	G	605	CHL	C3B-C4B	2.48	1.48	1.42
24	BE	605	CLA	C3B-C4B	2.48	1.48	1.42
24	C	512	CLA	MG-NB	-2.48	2.00	2.05
23	Au	601	CHL	C1D-ND	-2.48	1.34	1.37
26	BB	318	NEX	C12-C13	-2.48	1.40	1.45
23	9	605	CHL	C1B-C2B	2.48	1.49	1.43
34	h	102	DGD	O1G-C1G	-2.48	1.39	1.45
24	d	401	CLA	CMD-C2D	-2.48	1.45	1.50
24	G	611	CLA	MG-NB	-2.48	2.00	2.05
24	I	102	CLA	CMD-C2D	-2.48	1.45	1.50
23	0	605	CHL	C1B-C2B	2.48	1.49	1.43
24	b	617	CLA	C1B-C2B	2.48	1.49	1.43
23	N	605	CHL	C1B-NB	-2.48	1.34	1.37
24	B	609	CLA	C1B-C2B	2.48	1.49	1.43
24	A6	611	CLA	C1B-C2B	2.48	1.49	1.43
25	g	615	LUT	C32-C33	-2.48	1.40	1.45
26	BV	616	NEX	C10-C9	2.48	1.39	1.35
24	A6	613	CLA	C1B-C2B	2.48	1.49	1.43
23	y	306	CHL	C1B-NB	-2.48	1.34	1.37
25	AA	317	LUT	C28-C29	-2.48	1.40	1.45
24	1	508	CLA	C3B-C4B	2.48	1.48	1.42
24	BG	401	CLA	C1B-C2B	2.48	1.49	1.43
24	BF	514	CLA	MG-NB	-2.48	2.00	2.05
23	9	609	CHL	C3B-C4B	2.48	1.48	1.42
24	c	514	CLA	MG-NB	-2.48	2.00	2.05
24	6	603	CLA	C3B-C4B	2.48	1.48	1.42
23	Y	306	CHL	C1D-ND	-2.48	1.34	1.37
23	5	605	CHL	C1B-C2B	2.48	1.49	1.43
24	v	608	CLA	MG-NB	-2.48	2.00	2.05
24	Au	611	CLA	C1B-C2B	2.48	1.49	1.43
24	BU	612	CLA	C4B-NB	2.47	1.40	1.37
24	7	305	CLA	MG-NB	-2.47	2.00	2.05
24	AA	305	CLA	MG-NB	-2.47	2.00	2.05
24	B	604	CLA	C3B-C4B	2.47	1.48	1.42
24	9	613	CLA	C3B-C4B	2.47	1.48	1.42
23	S	601	CHL	C1B-NB	-2.47	1.34	1.37
24	7	303	CLA	C1B-C2B	2.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	613	CLA	C1B-C2B	2.47	1.49	1.43
24	1	503	CLA	C3B-C4B	2.47	1.48	1.42
25	BJ	615	LUT	C12-C13	-2.47	1.40	1.45
24	BE	605	CLA	C1B-C2B	2.47	1.49	1.43
24	C	507	CLA	MG-NB	-2.47	2.00	2.05
23	G	607	CHL	C3B-C4B	2.47	1.48	1.42
24	b	605	CLA	C3B-C4B	2.47	1.48	1.42
24	0	604	CLA	C3B-C4B	2.47	1.48	1.42
24	5	613	CLA	MG-NB	-2.47	2.00	2.05
24	BU	604	CLA	C4B-NB	2.47	1.40	1.37
24	B	611	CLA	C1B-C2B	2.47	1.49	1.43
24	B	604	CLA	MG-NB	-2.47	2.00	2.05
24	s	613	CLA	C1B-C2B	2.47	1.49	1.43
23	5	606	CHL	C4B-NB	-2.47	1.34	1.37
23	BJ	608	CHL	C4C-C3C	2.47	1.49	1.45
24	A	406	CLA	C1B-C2B	2.47	1.49	1.43
23	9	608	CHL	C1B-NB	-2.47	1.34	1.37
24	BV	604	CLA	CHC-C1C	2.47	1.43	1.38
23	Au	605	CHL	C4C-C3C	2.47	1.49	1.45
24	A2	612	CLA	C1B-C2B	2.47	1.49	1.43
23	r	606	CHL	C3B-C4B	2.47	1.48	1.42
24	S	608	CLA	C1B-C2B	2.47	1.49	1.43
24	A6	608	CLA	C1B-C2B	2.47	1.49	1.43
24	r	603	CLA	CMD-C2D	-2.47	1.45	1.50
34	BK	102	DGD	O1G-C1G	-2.47	1.39	1.45
24	d	401	CLA	C1B-C2B	2.46	1.49	1.43
24	Aw	102	CLA	C4B-NB	2.46	1.40	1.37
25	Y	316	LUT	C12-C13	-2.46	1.40	1.45
32	Az	101	SQD	O5-C1	2.46	1.48	1.41
23	BU	606	CHL	C3B-C4B	2.46	1.48	1.42
24	B	608	CLA	MG-NB	-2.46	2.00	2.05
23	AB	306	CHL	C3B-C4B	2.46	1.48	1.42
24	BF	511	CLA	C4B-NB	2.46	1.40	1.37
23	BJ	608	CHL	C1B-C2B	2.46	1.49	1.43
24	1	504	CLA	C1B-C2B	2.46	1.49	1.43
24	d	401	CLA	MG-NB	-2.46	2.00	2.05
24	B	616	CLA	C1B-C2B	2.46	1.49	1.43
23	S	607	CHL	C3B-C4B	2.46	1.48	1.42
24	BD	407	CLA	C1B-C2B	2.46	1.49	1.43
23	g	606	CHL	C3B-C4B	2.46	1.48	1.42
24	BU	603	CLA	CMD-C2D	-2.46	1.45	1.50
23	r	607	CHL	C1D-C2D	2.46	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BE	611	CLA	C1B-C2B	2.46	1.49	1.43
25	G	616	LUT	C28-C29	-2.46	1.40	1.45
24	C	504	CLA	C3B-C4B	2.46	1.48	1.42
24	Y	315	CLA	MG-NB	-2.46	2.00	2.05
23	g	608	CHL	C4C-C3C	2.46	1.49	1.45
23	s	606	CHL	C4C-C3C	2.46	1.49	1.45
25	N	616	LUT	C12-C13	-2.46	1.40	1.45
24	a	407	CLA	C1B-C2B	2.46	1.49	1.43
25	g	615	LUT	C12-C13	-2.46	1.40	1.45
24	Y	303	CLA	MG-NB	-2.46	2.00	2.05
24	BD	405	CLA	C3B-C4B	2.46	1.48	1.42
23	N	609	CHL	C3D-C2D	2.46	1.45	1.39
23	AA	306	CHL	C3B-C4B	2.46	1.48	1.42
23	5	609	CHL	C1B-NB	-2.46	1.34	1.37
23	8	305	CHL	C3B-C4B	2.46	1.48	1.42
23	9	607	CHL	C3B-C4B	2.46	1.48	1.42
23	BU	606	CHL	C1B-C2B	2.46	1.49	1.43
24	A	410	CLA	C1B-C2B	2.46	1.49	1.43
24	9	610	CLA	MG-NB	-2.46	2.00	2.05
23	r	613	CHL	MG-NA	-2.46	2.00	2.06
24	v	604	CLA	C3B-C4B	2.46	1.48	1.42
24	0	610	CLA	MG-NB	-2.46	2.00	2.05
25	BJ	615	LUT	C32-C33	-2.46	1.40	1.45
25	S	615	LUT	C32-C33	-2.46	1.40	1.45
25	A6	615	LUT	C32-C33	-2.46	1.40	1.45
23	Au	605	CHL	C3B-C4B	2.46	1.48	1.42
26	N	617	NEX	C32-C33	-2.46	1.40	1.45
24	I	102	CLA	C4B-NB	2.46	1.40	1.37
24	BE	613	CLA	C3B-C4B	2.46	1.48	1.42
25	A2	616	LUT	C12-C13	-2.46	1.40	1.45
24	R	405	CLA	C3B-C4B	2.46	1.48	1.42
23	8	304	CHL	C1B-C2B	2.46	1.49	1.43
24	BB	305	CLA	MG-NB	-2.46	2.00	2.05
24	R	405	CLA	C1B-C2B	2.45	1.49	1.43
24	C	510	CLA	MG-NB	-2.45	2.00	2.05
25	N	616	LUT	C32-C33	-2.45	1.40	1.45
24	1	506	CLA	C3B-C4B	2.45	1.48	1.42
24	BF	512	CLA	C3B-C4B	2.45	1.48	1.42
23	Y	309	CHL	C1B-NB	-2.45	1.34	1.37
24	6	613	CLA	CMB-C2B	-2.45	1.45	1.50
23	g	601	CHL	C1B-C2B	2.45	1.49	1.43
23	A2	606	CHL	C1D-ND	-2.45	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	MG-NB	-2.45	2.00	2.05
23	Au	608	CHL	C1B-NB	-2.45	1.34	1.37
24	v	602	CLA	C1B-C2B	2.45	1.49	1.43
25	BB	317	LUT	C12-C13	-2.45	1.40	1.45
23	Y	308	CHL	C1D-C2D	2.45	1.50	1.45
23	Ba	306	CHL	C3B-C4B	2.45	1.48	1.42
25	g	615	LUT	C28-C29	-2.45	1.40	1.45
24	S	611	CLA	C1B-C2B	2.45	1.49	1.43
23	5	605	CHL	C3B-C4B	2.45	1.48	1.42
24	AA	311	CLA	CMC-C2C	-2.45	1.45	1.50
23	g	607	CHL	C4C-C3C	2.45	1.49	1.45
24	BF	512	CLA	MG-NB	-2.45	2.00	2.05
24	0	612	CLA	CMD-C2D	-2.45	1.45	1.50
23	G	608	CHL	C1B-C2B	2.45	1.49	1.43
23	9	605	CHL	C3B-C4B	2.45	1.48	1.42
27	A2	618	LHG	O7-C5	-2.45	1.40	1.46
24	c	507	CLA	CMB-C2B	-2.45	1.45	1.50
23	r	606	CHL	C1B-C2B	2.45	1.49	1.43
24	AB	308	CLA	C4B-NB	2.45	1.40	1.37
23	A2	609	CHL	C1D-C2D	2.45	1.50	1.45
24	N	610	CLA	MG-NB	-2.45	2.00	2.05
23	Ba	308	CHL	C1B-C2B	2.45	1.49	1.43
23	6	601	CHL	MG-NA	-2.45	2.00	2.06
24	Aw	102	CLA	C3B-C4B	2.45	1.48	1.42
23	y	308	CHL	C1B-C2B	2.45	1.49	1.43
24	v	616	CLA	C1B-C2B	2.45	1.49	1.43
24	BB	311	CLA	C1B-C2B	2.45	1.49	1.43
25	7	316	LUT	C28-C29	-2.45	1.40	1.45
25	Ba	317	LUT	C12-C13	-2.45	1.40	1.45
24	6	610	CLA	CMC-C2C	-2.45	1.45	1.50
24	BB	314	CLA	C3B-C4B	2.44	1.48	1.42
23	n	609	CHL	C1B-C2B	2.44	1.49	1.43
24	BF	504	CLA	C3B-C4B	2.44	1.48	1.42
23	BU	607	CHL	C1D-C2D	2.44	1.50	1.45
24	c	509	CLA	MG-NB	-2.44	2.00	2.05
23	BU	613	CHL	C4B-NB	-2.44	1.34	1.37
23	7	309	CHL	C1B-C2B	2.44	1.49	1.43
23	BJ	606	CHL	C1B-C2B	2.44	1.49	1.43
24	C	507	CLA	C1B-C2B	2.44	1.49	1.43
34	1	516	DGD	O1G-C1G	-2.44	1.39	1.45
23	7	307	CHL	C1B-NB	-2.44	1.34	1.37
23	BU	605	CHL	C3D-C2D	2.44	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	608	CHL	C1D-C2D	2.44	1.50	1.45
23	BH	601	CHL	C1B-C2B	2.44	1.49	1.43
24	G	612	CLA	MG-NB	-2.44	2.00	2.05
23	g	606	CHL	C1B-C2B	2.44	1.49	1.43
25	y	317	LUT	C12-C13	-2.44	1.40	1.45
24	AB	310	CLA	MG-NB	-2.44	2.00	2.05
23	G	607	CHL	C1B-C2B	2.44	1.49	1.43
24	AB	310	CLA	C1B-C2B	2.44	1.49	1.43
23	r	607	CHL	C4C-C3C	2.44	1.49	1.45
24	BE	617	CLA	C1B-C2B	2.44	1.49	1.43
24	BF	512	CLA	CMB-C2B	-2.44	1.45	1.50
24	7	305	CLA	C1B-C2B	2.44	1.49	1.43
24	v	604	CLA	C1B-C2B	2.44	1.49	1.43
23	AA	307	CHL	C1B-NB	-2.44	1.34	1.37
23	AB	305	CHL	C3B-C4B	2.44	1.48	1.42
24	a	405	CLA	C3B-C4B	2.44	1.48	1.42
24	1	510	CLA	C1B-C2B	2.44	1.49	1.43
23	A2	609	CHL	C3D-C2D	2.44	1.45	1.39
24	AA	312	CLA	MG-NB	-2.44	2.01	2.05
24	b	611	CLA	C1B-C2B	2.44	1.49	1.43
24	1	513	CLA	C1B-C2B	2.44	1.49	1.43
24	a	405	CLA	MG-NB	-2.44	2.01	2.05
24	c	504	CLA	C1B-C2B	2.44	1.49	1.43
23	y	306	CHL	C3B-C4B	2.44	1.48	1.42
24	I	102	CLA	C3B-C4B	2.44	1.48	1.42
24	BE	614	CLA	C1B-C2B	2.44	1.49	1.43
24	y	312	CLA	C1B-C2B	2.44	1.49	1.43
24	BG	401	CLA	CMD-C2D	-2.44	1.45	1.50
24	7	312	CLA	MG-NB	-2.44	2.01	2.05
24	6	613	CLA	C1B-C2B	2.44	1.49	1.43
24	r	603	CLA	C1B-C2B	2.44	1.49	1.43
25	BB	316	LUT	C28-C29	-2.44	1.40	1.45
26	BB	318	NEX	C28-C29	-2.44	1.40	1.45
26	5	617	NEX	C28-C29	-2.44	1.40	1.45
23	N	609	CHL	C1D-ND	-2.44	1.34	1.37
24	AB	308	CLA	C1D-ND	2.44	1.40	1.37
24	BD	410	CLA	MG-NB	-2.43	2.01	2.05
24	c	506	CLA	C1B-C2B	2.43	1.49	1.43
26	Y	318	NEX	C28-C29	-2.43	1.40	1.45
24	c	503	CLA	C1B-C2B	2.43	1.49	1.43
23	6	609	CHL	C1C-NC	-2.43	1.34	1.37
34	C	516	DGD	O1G-C1G	-2.43	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Aw	102	CLA	CMD-C2D	-2.43	1.45	1.50
24	a	410	CLA	MG-NB	-2.43	2.01	2.05
24	AA	304	CLA	MG-NB	-2.43	2.01	2.05
25	Y	317	LUT	C12-C13	-2.43	1.40	1.45
23	BU	607	CHL	C4C-C3C	2.43	1.49	1.45
24	Au	612	CLA	MG-NB	-2.43	2.01	2.05
23	7	307	CHL	C1B-C2B	2.43	1.49	1.43
24	BU	610	CLA	C1B-C2B	2.43	1.49	1.43
23	Au	609	CHL	C4B-NB	-2.43	1.34	1.37
24	BB	305	CLA	C1B-C2B	2.43	1.49	1.43
25	A2	615	LUT	C12-C13	-2.43	1.40	1.45
23	s	607	CHL	MG-NA	-2.43	2.00	2.06
23	9	605	CHL	C1B-NB	-2.43	1.34	1.37
23	AB	306	CHL	C1D-C2D	2.43	1.50	1.45
23	BU	605	CHL	C1B-C2B	2.43	1.49	1.43
23	BB	309	CHL	C1B-NB	-2.43	1.34	1.37
24	BF	513	CLA	C3B-C4B	2.43	1.48	1.42
24	8	302	CLA	MG-NB	-2.43	2.01	2.05
28	G	619	XAT	C18-C5	2.43	1.55	1.51
24	r	602	CLA	CMC-C2C	-2.43	1.45	1.50
24	BF	508	CLA	CMD-C2D	-2.43	1.45	1.50
25	n	616	LUT	C12-C13	-2.43	1.40	1.45
23	BQ	605	CHL	C3B-C4B	2.43	1.48	1.42
24	BF	510	CLA	C1B-NB	-2.43	1.34	1.37
25	BJ	615	LUT	C28-C29	-2.43	1.40	1.45
24	C	509	CLA	C1B-C2B	2.43	1.49	1.43
26	9	617	NEX	C28-C29	-2.43	1.40	1.45
24	A	405	CLA	MG-NB	-2.43	2.01	2.05
24	c	512	CLA	CMB-C2B	-2.43	1.45	1.50
24	B	610	CLA	C1B-C2B	2.43	1.49	1.43
23	0	601	CHL	MG-NA	-2.43	2.00	2.06
25	S	614	LUT	C32-C33	-2.43	1.40	1.45
25	AA	317	LUT	C12-C13	-2.43	1.40	1.45
26	BB	318	NEX	C32-C33	-2.43	1.40	1.45
23	BJ	606	CHL	C3B-C4B	2.43	1.48	1.42
24	N	612	CLA	C1B-C2B	2.43	1.49	1.43
23	Ba	308	CHL	C4C-C3C	2.43	1.49	1.45
23	BB	307	CHL	C1D-ND	-2.42	1.34	1.37
24	1	507	CLA	C1B-C2B	2.42	1.49	1.43
24	BD	410	CLA	C1B-C2B	2.42	1.49	1.43
27	Y	319	LHG	O7-C5	-2.42	1.40	1.46
23	BV	607	CHL	MG-NA	-2.42	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	316	LUT	C28-C29	-2.42	1.40	1.45
24	D	401	CLA	CMD-C2D	-2.42	1.45	1.50
23	BV	606	CHL	C4C-C3C	2.42	1.49	1.45
25	y	316	LUT	C28-C29	-2.42	1.40	1.45
25	7	317	LUT	C12-C13	-2.42	1.40	1.45
24	G	604	CLA	C1B-C2B	2.42	1.49	1.43
23	7	309	CHL	C4C-C3C	2.42	1.49	1.45
24	N	603	CLA	MG-NB	-2.42	2.01	2.05
24	A2	603	CLA	MG-NB	-2.42	2.01	2.05
24	7	304	CLA	MG-NB	-2.42	2.01	2.05
24	BD	407	CLA	MG-NB	-2.42	2.01	2.05
24	B	603	CLA	C1B-C2B	2.42	1.49	1.43
24	B	612	CLA	C3B-C4B	2.42	1.48	1.42
34	BD	401	DGD	O2G-C2G	-2.42	1.40	1.46
24	B	613	CLA	MG-NB	-2.42	2.01	2.05
24	BU	602	CLA	C1B-NB	-2.42	1.34	1.37
25	7	317	LUT	C28-C29	-2.42	1.40	1.45
23	8	306	CHL	C3B-C4B	2.42	1.48	1.42
25	BV	615	LUT	C12-C13	-2.42	1.40	1.45
23	y	308	CHL	C4C-C3C	2.42	1.49	1.45
23	A2	605	CHL	C1B-NB	-2.42	1.34	1.37
23	8	305	CHL	MG-NA	-2.42	2.00	2.06
26	r	617	NEX	C12-C13	-2.42	1.40	1.45
24	R	404	CLA	MG-NB	-2.42	2.01	2.05
24	BD	406	CLA	C3B-C4B	2.42	1.48	1.42
23	g	609	CHL	C1B-C2B	2.42	1.49	1.43
23	N	606	CHL	C3B-C4B	2.42	1.48	1.42
23	Au	601	CHL	MG-NA	-2.42	2.00	2.06
23	S	607	CHL	C1D-ND	-2.42	1.34	1.37
23	n	605	CHL	C3B-C4B	2.42	1.48	1.42
24	Y	303	CLA	CMB-C2B	-2.42	1.45	1.50
23	Y	306	CHL	C1B-C2B	2.42	1.48	1.43
24	v	603	CLA	C1B-C2B	2.42	1.48	1.43
24	R	409	CLA	C1B-C2B	2.42	1.48	1.43
24	A	406	CLA	CMD-C2D	-2.42	1.45	1.50
24	BB	304	CLA	MG-NB	-2.42	2.01	2.05
24	BF	509	CLA	MG-NB	-2.42	2.01	2.05
23	N	606	CHL	C1D-ND	-2.42	1.34	1.37
23	BQ	605	CHL	C1B-C2B	2.42	1.48	1.43
24	AA	311	CLA	C1B-C2B	2.42	1.48	1.43
23	n	608	CHL	MG-NA	-2.42	2.00	2.06
24	D	401	CLA	MG-NB	-2.42	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BB	317	LUT	C28-C29	-2.41	1.40	1.45
24	G	603	CLA	C1B-C2B	2.41	1.48	1.43
24	b	612	CLA	C1B-C2B	2.41	1.48	1.43
28	Au	619	XAT	C18-C5	2.41	1.55	1.51
26	N	617	NEX	C28-C29	-2.41	1.40	1.45
23	BJ	601	CHL	C1B-C2B	2.41	1.48	1.43
24	A	407	CLA	C1B-C2B	2.41	1.48	1.43
26	r	617	NEX	C28-C29	-2.41	1.40	1.45
24	v	604	CLA	CMB-C2B	-2.41	1.45	1.50
23	5	607	CHL	MG-NA	-2.41	2.00	2.06
24	BE	607	CLA	C1B-C2B	2.41	1.48	1.43
24	BG	402	CLA	MG-NB	-2.41	2.01	2.05
24	BB	304	CLA	CMB-C2B	-2.41	1.45	1.50
23	6	606	CHL	C3B-C4B	2.41	1.48	1.42
34	a	401	DGD	O2G-C2G	-2.41	1.40	1.46
24	Au	611	CLA	MG-NB	-2.41	2.01	2.05
24	a	410	CLA	C1B-C2B	2.41	1.48	1.43
23	BB	302	CHL	C3B-C4B	2.41	1.48	1.42
24	BQ	610	CLA	CHC-C1C	2.41	1.43	1.38
24	G	610	CLA	MG-NB	-2.41	2.01	2.05
23	G	608	CHL	C3B-C4B	2.41	1.48	1.42
24	Y	305	CLA	MG-NB	-2.41	2.01	2.05
31	D	403	PL9	C7-C8	-2.41	1.47	1.50
23	AA	309	CHL	C1B-C2B	2.41	1.48	1.43
23	BJ	609	CHL	C1B-C2B	2.41	1.48	1.43
26	BB	320	NEX	C12-C13	-2.41	1.40	1.45
23	BJ	607	CHL	C4C-C3C	2.41	1.49	1.45
23	e	601	CHL	C1B-C2B	2.41	1.48	1.43
23	n	605	CHL	C1B-C2B	2.41	1.48	1.43
24	BE	605	CLA	MG-NB	-2.41	2.01	2.05
23	9	607	CHL	MG-NA	-2.41	2.00	2.06
23	N	601	CHL	C4B-NB	-2.41	1.34	1.37
23	r	605	CHL	C1B-C2B	2.41	1.48	1.43
23	N	607	CHL	C3B-C4B	2.41	1.48	1.42
23	N	601	CHL	C1B-NB	-2.41	1.34	1.37
23	Au	608	CHL	C1B-C2B	2.41	1.48	1.43
24	c	513	CLA	C1B-C2B	2.41	1.48	1.43
24	AA	303	CLA	C1B-C2B	2.41	1.48	1.43
23	G	601	CHL	C3B-C4B	2.41	1.48	1.42
27	2	406	LHG	O7-C5	-2.41	1.40	1.46
24	S	613	CLA	MG-NB	-2.41	2.01	2.05
24	Y	315	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Av	102	DGD	O2G-C2G	-2.41	1.40	1.46
23	BV	601	CHL	C1B-NB	-2.41	1.34	1.37
23	BU	613	CHL	C3B-C4B	2.41	1.48	1.42
24	9	604	CLA	CHC-C1C	2.41	1.43	1.38
23	6	605	CHL	C1B-NB	-2.41	1.34	1.37
23	y	306	CHL	C4B-NB	-2.41	1.34	1.37
23	Ba	302	CHL	C1B-NB	-2.41	1.34	1.37
23	AA	309	CHL	C4C-C3C	2.41	1.49	1.45
24	b	613	CLA	MG-NB	-2.41	2.01	2.05
31	D	403	PL9	C5-C4	-2.41	1.38	1.47
23	A6	606	CHL	C1B-NB	-2.41	1.34	1.37
23	5	607	CHL	C1D-C2D	2.41	1.50	1.45
24	Y	313	CLA	C1B-C2B	2.41	1.48	1.43
24	c	511	CLA	C1B-C2B	2.41	1.48	1.43
24	1	511	CLA	MG-NB	-2.40	2.01	2.05
24	1	513	CLA	MG-NB	-2.40	2.01	2.05
38	a	408	PHO	C4D-ND	-2.40	1.35	1.38
24	C	506	CLA	MG-NB	-2.40	2.01	2.05
24	Y	305	CLA	CMB-C2B	-2.40	1.45	1.50
26	A6	616	NEX	C32-C33	-2.40	1.40	1.45
23	BV	605	CHL	C1B-C2B	2.40	1.48	1.43
23	0	609	CHL	C4C-C3C	2.40	1.49	1.45
25	A2	615	LUT	C28-C29	-2.40	1.40	1.45
24	Au	603	CLA	CMD-C2D	-2.40	1.45	1.50
23	S	606	CHL	C1B-C2B	2.40	1.48	1.43
24	BU	603	CLA	C1B-C2B	2.40	1.48	1.43
25	0	615	LUT	C12-C13	-2.40	1.40	1.45
24	A6	611	CLA	MG-NB	-2.40	2.01	2.05
24	BD	405	CLA	MG-NB	-2.40	2.01	2.05
24	s	602	CLA	CHC-C1C	2.40	1.43	1.38
23	Y	309	CHL	C1B-C2B	2.40	1.48	1.43
24	AA	305	CLA	C1B-C2B	2.40	1.48	1.43
24	BF	512	CLA	C1B-C2B	2.40	1.48	1.43
23	g	606	CHL	C4C-C3C	2.40	1.49	1.45
24	9	603	CLA	C1B-C2B	2.40	1.48	1.43
26	A2	617	NEX	C28-C29	-2.40	1.40	1.45
23	s	605	CHL	C4C-C3C	2.40	1.49	1.45
24	C	509	CLA	C3B-C4B	2.40	1.48	1.42
23	S	607	CHL	C1B-C2B	2.40	1.48	1.43
24	A6	604	CLA	MG-NB	-2.40	2.01	2.05
24	BF	504	CLA	MG-NB	-2.40	2.01	2.05
26	Y	318	NEX	C12-C13	-2.40	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C3B-C4B	2.40	1.48	1.42
24	C	504	CLA	MG-NB	-2.40	2.01	2.05
24	a	407	CLA	MG-NB	-2.40	2.01	2.05
24	BF	506	CLA	C1B-C2B	2.40	1.48	1.43
25	BQ	616	LUT	C32-C33	-2.40	1.40	1.45
23	AA	302	CHL	C4C-C3C	2.40	1.49	1.45
23	AA	307	CHL	C1B-C2B	2.40	1.48	1.43
26	BB	320	NEX	C28-C29	-2.40	1.40	1.45
24	b	607	CLA	C1B-C2B	2.40	1.48	1.43
23	AB	305	CHL	MG-NA	-2.40	2.00	2.06
23	8	307	CHL	C4B-NB	-2.40	1.34	1.37
24	BF	504	CLA	C1B-C2B	2.40	1.48	1.43
24	v	615	CLA	MG-NB	-2.40	2.01	2.05
24	Aw	102	CLA	CMB-C2B	-2.40	1.45	1.50
23	A6	606	CHL	C3B-C4B	2.40	1.48	1.42
23	G	601	CHL	C1D-ND	-2.40	1.34	1.37
24	B	616	CLA	CMC-C2C	-2.40	1.45	1.50
24	BF	509	CLA	CMB-C2B	-2.40	1.45	1.50
24	v	613	CLA	MG-NB	-2.40	2.01	2.05
23	8	304	CHL	C3B-C4B	2.40	1.48	1.42
26	S	616	NEX	C32-C33	-2.40	1.40	1.45
24	Ba	312	CLA	C1B-C2B	2.40	1.48	1.43
23	8	307	CHL	MG-NA	-2.40	2.00	2.06
23	A2	606	CHL	C3B-C4B	2.40	1.48	1.42
24	r	612	CLA	C3B-C4B	2.40	1.48	1.42
24	C	511	CLA	MG-ND	-2.40	2.01	2.05
24	v	612	CLA	C3B-C4B	2.39	1.48	1.42
24	c	508	CLA	C4B-NB	2.39	1.40	1.37
25	AA	316	LUT	C28-C29	-2.39	1.40	1.45
24	R	406	CLA	C1B-C2B	2.39	1.48	1.43
24	A	407	CLA	MG-NB	-2.39	2.01	2.05
25	N	615	LUT	C28-C29	-2.39	1.40	1.45
24	AA	312	CLA	C1B-C2B	2.39	1.48	1.43
23	BB	309	CHL	MG-NA	-2.39	2.00	2.06
24	AA	313	CLA	CMD-C2D	-2.39	1.45	1.50
26	9	617	NEX	C12-C13	-2.39	1.40	1.45
24	A2	604	CLA	MG-NB	-2.39	2.01	2.05
23	A2	601	CHL	C3B-C4B	2.39	1.48	1.42
34	R	401	DGD	O2G-C2G	-2.39	1.40	1.46
24	6	614	CLA	C1B-C2B	2.39	1.48	1.43
24	7	312	CLA	C1B-C2B	2.39	1.48	1.43
24	r	609	CLA	CMC-C2C	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	610	CLA	C1B-C2B	2.39	1.48	1.43
34	c	516	DGD	O1G-C1G	-2.39	1.39	1.45
23	Y	309	CHL	C1D-C2D	2.39	1.50	1.45
25	n	616	LUT	C32-C33	-2.39	1.40	1.45
23	y	302	CHL	C1B-NB	-2.39	1.34	1.37
23	0	605	CHL	C1D-ND	-2.39	1.34	1.37
23	BB	302	CHL	C1B-NB	-2.39	1.34	1.37
25	A6	615	LUT	C12-C13	-2.39	1.40	1.45
24	6	612	CLA	CMD-C2D	-2.39	1.45	1.50
23	8	305	CHL	C4B-NB	-2.39	1.34	1.37
24	v	610	CLA	C1B-C2B	2.39	1.48	1.43
24	y	313	CLA	CMD-C2D	-2.39	1.45	1.50
24	c	512	CLA	MG-NB	-2.39	2.01	2.05
23	y	302	CHL	MG-NA	-2.39	2.00	2.06
23	BB	308	CHL	C1D-ND	-2.39	1.34	1.37
24	1	503	CLA	CMB-C2B	-2.39	1.45	1.50
24	0	611	CLA	MG-NB	-2.39	2.01	2.05
23	5	608	CHL	C3B-C4B	2.39	1.48	1.42
23	r	607	CHL	C3B-C4B	2.39	1.48	1.42
24	1	504	CLA	C3B-C4B	2.39	1.48	1.42
23	A6	607	CHL	C1B-C2B	2.39	1.48	1.43
24	2	402	CLA	CMD-C2D	-2.39	1.45	1.50
25	BV	615	LUT	C32-C33	-2.39	1.40	1.45
23	0	607	CHL	C4C-C3C	2.39	1.49	1.45
24	v	605	CLA	MG-NB	-2.39	2.01	2.05
24	0	614	CLA	C1B-C2B	2.39	1.48	1.43
24	B	610	CLA	MG-NB	-2.39	2.01	2.05
24	A6	609	CLA	MG-NB	-2.39	2.01	2.05
24	BD	406	CLA	MG-NB	-2.39	2.01	2.05
23	G	608	CHL	C4B-NB	-2.39	1.34	1.37
24	BF	513	CLA	C1B-C2B	2.39	1.48	1.43
23	BU	613	CHL	MG-NA	-2.39	2.00	2.06
24	c	510	CLA	C1B-C2B	2.39	1.48	1.43
24	5	604	CLA	CHC-C1C	2.38	1.43	1.38
23	y	302	CHL	C1B-C2B	2.38	1.48	1.43
23	A2	607	CHL	C1D-ND	-2.38	1.34	1.37
23	0	601	CHL	C4C-C3C	2.38	1.49	1.45
24	c	514	CLA	C1B-C2B	2.38	1.48	1.43
23	6	608	CHL	C3B-C4B	2.38	1.48	1.42
24	Au	610	CLA	MG-NB	-2.38	2.01	2.05
27	b	623	LHG	O7-C5	-2.38	1.40	1.46
24	B	613	CLA	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	C1B-C2B	2.38	1.48	1.43
23	Y	302	CHL	C1B-NB	-2.38	1.34	1.37
25	Ba	316	LUT	C12-C13	-2.38	1.40	1.45
23	AA	306	CHL	C1B-NB	-2.38	1.34	1.37
23	BJ	606	CHL	C4C-C3C	2.38	1.49	1.45
24	v	609	CLA	MG-NB	-2.38	2.01	2.05
24	BU	609	CLA	C1B-C2B	2.38	1.48	1.43
23	0	605	CHL	C1B-NB	-2.38	1.34	1.37
24	d	402	CLA	MG-NB	-2.38	2.01	2.05
25	A2	616	LUT	C28-C29	-2.38	1.40	1.45
24	B	615	CLA	MG-NB	-2.38	2.01	2.05
24	AB	301	CLA	MG-NB	-2.38	2.01	2.05
24	A2	602	CLA	MG-NB	-2.38	2.01	2.05
24	v	611	CLA	C1B-C2B	2.38	1.48	1.43
24	6	611	CLA	MG-NB	-2.38	2.01	2.05
23	AA	307	CHL	MG-NA	-2.38	2.00	2.06
23	S	606	CHL	C3B-C4B	2.38	1.48	1.42
23	BU	607	CHL	C3B-C4B	2.38	1.48	1.42
24	S	611	CLA	MG-NB	-2.38	2.01	2.05
25	9	616	LUT	C32-C33	-2.38	1.40	1.45
25	Ba	316	LUT	C28-C29	-2.38	1.40	1.45
24	c	504	CLA	MG-NB	-2.38	2.01	2.05
24	v	610	CLA	MG-NB	-2.38	2.01	2.05
23	N	608	CHL	C1B-C2B	2.38	1.48	1.43
24	8	308	CLA	C1B-C2B	2.38	1.48	1.43
34	H	102	DGD	O2G-C2G	-2.38	1.40	1.46
24	BF	506	CLA	MG-NB	-2.38	2.01	2.05
24	C	503	CLA	C1B-C2B	2.38	1.48	1.43
24	BE	612	CLA	C1B-C2B	2.38	1.48	1.43
23	s	605	CHL	C1B-C2B	2.38	1.48	1.43
24	G	602	CLA	C1B-C2B	2.38	1.48	1.43
23	8	304	CHL	C1B-NB	-2.38	1.34	1.37
23	AB	305	CHL	C1D-ND	-2.38	1.34	1.37
24	0	612	CLA	MG-NB	-2.38	2.01	2.05
25	s	615	LUT	C12-C13	-2.38	1.40	1.45
24	BF	511	CLA	CMD-C2D	-2.38	1.45	1.50
23	r	613	CHL	C1D-ND	-2.38	1.34	1.37
23	A2	601	CHL	C1B-NB	-2.38	1.34	1.37
24	1	506	CLA	MG-NB	-2.38	2.01	2.05
23	r	613	CHL	C3B-C4B	2.38	1.48	1.42
24	BU	611	CLA	CMD-C2D	-2.38	1.45	1.50
23	BQ	607	CHL	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Ba	306	CHL	C4B-NB	-2.38	1.34	1.37
28	Y	301	XAT	C18-C5	2.38	1.55	1.51
23	G	601	CHL	C1B-C2B	2.37	1.48	1.43
24	c	503	CLA	CMB-C2B	-2.37	1.45	1.50
24	BV	602	CLA	CHC-C1C	2.37	1.43	1.38
23	8	305	CHL	C1B-C2B	2.37	1.48	1.43
24	6	612	CLA	MG-NB	-2.37	2.01	2.05
24	R	406	CLA	MG-NB	-2.37	2.01	2.05
23	6	606	CHL	C1D-ND	-2.37	1.34	1.37
23	Au	601	CHL	C1B-C2B	2.37	1.48	1.43
24	c	506	CLA	MG-NB	-2.37	2.01	2.05
23	BQ	608	CHL	MG-NA	-2.37	2.00	2.06
23	Y	310	CHL	C3B-C4B	2.37	1.48	1.42
25	BQ	615	LUT	C12-C13	-2.37	1.40	1.45
23	6	601	CHL	C4B-NB	-2.37	1.34	1.37
23	Y	308	CHL	C1D-ND	-2.37	1.34	1.37
24	G	613	CLA	MG-NB	-2.37	2.01	2.05
38	R	408	PHO	C3B-C2B	-2.37	1.37	1.40
23	0	601	CHL	C4B-NB	-2.37	1.34	1.37
24	v	616	CLA	CMC-C2C	-2.37	1.45	1.50
24	BB	311	CLA	CMC-C2C	-2.37	1.45	1.50
24	N	604	CLA	MG-NB	-2.37	2.01	2.05
24	BF	510	CLA	C1B-C2B	2.37	1.48	1.43
27	B	622	LHG	O7-C5	-2.37	1.40	1.46
24	A2	612	CLA	MG-NB	-2.37	2.01	2.05
23	AA	302	CHL	C4B-NB	-2.37	1.34	1.37
24	6	602	CLA	CMB-C2B	-2.37	1.45	1.50
24	1	505	CLA	MG-NB	-2.37	2.01	2.05
24	BF	502	CLA	CMD-C2D	-2.37	1.45	1.50
23	N	601	CHL	C3B-C4B	2.37	1.48	1.42
24	BE	608	CLA	MG-NB	-2.37	2.01	2.05
24	6	613	CLA	CMD-C2D	-2.37	1.45	1.50
23	n	609	CHL	MG-NA	-2.37	2.00	2.06
23	9	607	CHL	C1D-C2D	2.37	1.50	1.45
24	5	602	CLA	C1B-C2B	2.37	1.48	1.43
24	Au	603	CLA	C1B-C2B	2.37	1.48	1.43
23	AA	308	CHL	C1D-ND	-2.37	1.34	1.37
25	G	616	LUT	C12-C13	-2.37	1.40	1.45
26	Y	318	NEX	C32-C33	-2.37	1.40	1.45
24	b	614	CLA	MG-NB	-2.37	2.01	2.05
24	BE	614	CLA	MG-NB	-2.37	2.01	2.05
24	v	606	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	605	CHL	C1D-ND	-2.37	1.34	1.37
23	Ba	302	CHL	C1B-C2B	2.37	1.48	1.43
24	N	603	CLA	C1B-C2B	2.37	1.48	1.43
24	BF	511	CLA	C1B-C2B	2.37	1.48	1.43
23	G	608	CHL	C1B-NB	-2.37	1.34	1.37
24	r	602	CLA	C1B-NB	-2.37	1.34	1.37
23	BB	306	CHL	C1B-C2B	2.37	1.48	1.43
24	R	405	CLA	MG-NB	-2.37	2.01	2.05
24	Au	604	CLA	C1B-C2B	2.37	1.48	1.43
24	v	608	CLA	CMB-C2B	-2.37	1.45	1.50
23	8	304	CHL	C4B-NB	-2.37	1.34	1.37
24	N	612	CLA	MG-NB	-2.37	2.01	2.05
24	A2	602	CLA	CMB-C2B	-2.36	1.45	1.50
24	8	301	CLA	MG-NB	-2.36	2.01	2.05
24	v	607	CLA	MG-NB	-2.36	2.01	2.05
24	BV	613	CLA	MG-NB	-2.36	2.01	2.05
25	s	614	LUT	C28-C29	-2.36	1.40	1.45
23	y	306	CHL	C1B-C2B	2.36	1.48	1.43
24	BF	509	CLA	C1B-C2B	2.36	1.48	1.43
23	BB	309	CHL	C1D-C2D	2.36	1.50	1.45
24	A6	602	CLA	MG-NB	-2.36	2.01	2.05
23	A2	608	CHL	C1B-C2B	2.36	1.48	1.43
24	v	611	CLA	CMB-C2B	-2.36	1.45	1.50
23	G	609	CHL	C1B-C2B	2.36	1.48	1.43
24	Au	610	CLA	C1B-C2B	2.36	1.48	1.43
24	A2	602	CLA	C1B-C2B	2.36	1.48	1.43
24	B	605	CLA	MG-NB	-2.36	2.01	2.05
24	AA	314	CLA	MG-NB	-2.36	2.01	2.05
23	r	613	CHL	C4B-NB	-2.36	1.34	1.37
24	BE	611	CLA	MG-NB	-2.36	2.01	2.05
24	v	608	CLA	C1B-C2B	2.36	1.48	1.43
23	Y	309	CHL	MG-NA	-2.36	2.00	2.06
23	Ba	302	CHL	MG-NA	-2.36	2.00	2.06
24	S	604	CLA	MG-NB	-2.36	2.01	2.05
23	G	606	CHL	C3B-C4B	2.36	1.48	1.42
24	Y	304	CLA	C1B-C2B	2.36	1.48	1.43
24	BE	613	CLA	CMD-C2D	-2.36	1.45	1.50
24	r	609	CLA	C1B-NB	-2.36	1.34	1.37
25	Y	317	LUT	C28-C29	-2.36	1.40	1.45
23	6	606	CHL	C1D-C2D	2.36	1.50	1.45
23	BQ	606	CHL	C3B-C4B	2.36	1.48	1.42
24	R	404	CLA	CMD-C2D	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	0	607	CHL	C1D-ND	-2.36	1.34	1.37
23	BB	308	CHL	C4B-NB	-2.36	1.34	1.37
23	BU	605	CHL	CHC-C4B	2.36	1.44	1.39
28	BB	301	XAT	C18-C5	2.36	1.55	1.51
23	BQ	609	CHL	MG-NA	-2.36	2.00	2.06
33	F	102	HEM	FE-NA	2.36	2.03	1.95
25	BQ	615	LUT	C32-C33	-2.36	1.40	1.45
23	A6	606	CHL	C1B-C2B	2.36	1.48	1.43
24	r	609	CLA	C1B-C2B	2.36	1.48	1.43
24	r	611	CLA	CMD-C2D	-2.36	1.45	1.50
25	y	317	LUT	C32-C33	-2.36	1.40	1.45
23	A2	607	CHL	C4B-NB	-2.36	1.34	1.37
23	r	605	CHL	C1D-C2D	2.36	1.50	1.45
23	0	606	CHL	C3B-C4B	2.36	1.48	1.42
24	s	604	CLA	CHC-C1C	2.36	1.43	1.38
24	I	102	CLA	CMB-C2B	-2.36	1.45	1.50
23	AA	307	CHL	C4B-NB	-2.36	1.34	1.37
24	BF	508	CLA	C4B-NB	2.36	1.40	1.37
25	s	614	LUT	C12-C13	-2.36	1.40	1.45
25	s	615	LUT	C32-C33	-2.36	1.40	1.45
24	N	602	CLA	C1B-C2B	2.36	1.48	1.43
27	N	618	LHG	O7-C5	-2.36	1.40	1.46
23	BQ	609	CHL	C1B-C2B	2.36	1.48	1.43
24	1	503	CLA	C1B-C2B	2.36	1.48	1.43
24	Au	614	CLA	MG-NB	-2.36	2.01	2.05
24	A6	613	CLA	MG-NB	-2.36	2.01	2.05
24	G	610	CLA	C1B-C2B	2.35	1.48	1.43
25	Au	615	LUT	C28-C29	-2.35	1.40	1.45
23	BB	308	CHL	C1D-C2D	2.35	1.50	1.45
25	n	615	LUT	C12-C13	-2.35	1.40	1.45
23	BJ	601	CHL	C4C-C3C	2.35	1.49	1.45
23	n	606	CHL	C3B-C4B	2.35	1.48	1.42
24	b	609	CLA	MG-NB	-2.35	2.01	2.05
24	s	613	CLA	MG-NB	-2.35	2.01	2.05
23	BB	309	CHL	C1B-C2B	2.35	1.48	1.43
24	0	613	CLA	CMD-C2D	-2.35	1.45	1.50
24	Ba	313	CLA	CMD-C2D	-2.35	1.45	1.50
24	1	508	CLA	CMB-C2B	-2.35	1.45	1.50
23	BB	310	CHL	C3B-C4B	2.35	1.48	1.42
26	A6	616	NEX	C28-C29	-2.35	1.40	1.45
23	Y	307	CHL	C1D-C2D	2.35	1.50	1.45
24	S	602	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	308	CHL	C4B-NB	-2.35	1.34	1.37
23	AB	305	CHL	C4B-NB	-2.35	1.34	1.37
25	S	615	LUT	C12-C13	-2.35	1.40	1.45
24	R	405	CLA	CMD-C2D	-2.35	1.45	1.50
24	7	314	CLA	MG-NB	-2.35	2.01	2.05
24	b	608	CLA	MG-NB	-2.35	2.01	2.05
24	BU	604	CLA	C1B-NB	-2.35	1.34	1.37
24	C	512	CLA	C1B-C2B	2.35	1.48	1.43
24	BF	510	CLA	CMD-C2D	-2.35	1.45	1.50
24	BU	610	CLA	CMD-C2D	-2.35	1.45	1.50
25	y	316	LUT	C12-C13	-2.35	1.40	1.45
23	S	605	CHL	C1B-C2B	2.35	1.48	1.43
24	BF	503	CLA	C1B-C2B	2.35	1.48	1.43
24	BB	313	CLA	CMD-C2D	-2.35	1.45	1.50
23	BV	605	CHL	C4C-C3C	2.35	1.49	1.45
24	N	610	CLA	CMC-C2C	-2.35	1.45	1.50
24	BB	311	CLA	CMB-C2B	-2.35	1.45	1.50
24	c	502	CLA	CMD-C2D	-2.35	1.45	1.50
23	s	601	CHL	C1B-NB	-2.35	1.34	1.37
28	7	301	XAT	C18-C5	2.35	1.55	1.51
23	N	608	CHL	C3B-C4B	2.35	1.48	1.42
23	0	608	CHL	C3B-C4B	2.35	1.48	1.42
23	A2	608	CHL	C3B-C4B	2.35	1.48	1.42
24	c	510	CLA	C1B-NB	-2.35	1.34	1.37
24	BU	604	CLA	CMD-C2D	-2.35	1.45	1.50
25	BQ	616	LUT	C12-C13	-2.35	1.40	1.45
26	9	617	NEX	C32-C33	-2.35	1.40	1.45
23	A2	601	CHL	C1B-C2B	2.35	1.48	1.43
24	A	406	CLA	MG-NB	-2.35	2.01	2.05
24	2	403	CLA	MG-NB	-2.35	2.01	2.05
23	7	306	CHL	C1B-NB	-2.35	1.34	1.37
24	r	611	CLA	C1B-C2B	2.35	1.48	1.43
23	9	606	CHL	MG-NA	-2.35	2.00	2.06
24	BE	609	CLA	MG-NB	-2.35	2.01	2.05
24	1	504	CLA	MG-NB	-2.35	2.01	2.05
23	6	609	CHL	C1B-C2B	2.35	1.48	1.43
23	5	608	CHL	C1B-C2B	2.35	1.48	1.43
24	5	612	CLA	C1B-C2B	2.35	1.48	1.43
25	BV	614	LUT	C32-C33	-2.35	1.40	1.45
24	8	310	CLA	MG-NB	-2.35	2.01	2.05
24	N	602	CLA	MG-NB	-2.35	2.01	2.05
23	BB	307	CHL	C1D-C2D	2.34	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C1B-C2B	2.34	1.48	1.43
25	G	616	LUT	C32-C33	-2.34	1.40	1.45
23	8	307	CHL	C1D-ND	-2.34	1.34	1.37
23	y	309	CHL	C1B-NB	-2.34	1.34	1.37
25	s	614	LUT	C32-C33	-2.34	1.40	1.45
25	0	616	LUT	C28-C29	-2.34	1.40	1.45
24	v	611	CLA	CMC-C2C	-2.34	1.45	1.50
23	n	608	CHL	C4C-C3C	2.34	1.49	1.45
23	7	308	CHL	C1D-ND	-2.34	1.34	1.37
23	Y	306	CHL	C3B-C4B	2.34	1.48	1.42
23	6	601	CHL	C4C-C3C	2.34	1.49	1.45
24	BE	612	CLA	CMD-C2D	-2.34	1.45	1.50
23	Au	608	CHL	C4B-NB	-2.34	1.34	1.37
23	G	608	CHL	C1D-ND	-2.34	1.34	1.37
23	y	309	CHL	C4B-NB	-2.34	1.34	1.37
23	BB	302	CHL	C1D-ND	-2.34	1.34	1.37
25	N	616	LUT	C28-C29	-2.34	1.40	1.45
23	n	607	CHL	C1B-C2B	2.34	1.48	1.43
23	A2	601	CHL	C4B-NB	-2.34	1.34	1.37
23	N	601	CHL	C1B-C2B	2.34	1.48	1.43
25	Ba	317	LUT	C32-C33	-2.34	1.40	1.45
23	Y	307	CHL	C1D-ND	-2.34	1.34	1.37
23	9	605	CHL	C1D-ND	-2.34	1.34	1.37
23	BQ	609	CHL	C1B-NB	-2.34	1.34	1.37
23	G	601	CHL	MG-NA	-2.34	2.00	2.06
24	r	604	CLA	C1B-C2B	2.34	1.48	1.43
24	A6	602	CLA	C1B-C2B	2.34	1.48	1.43
24	Y	304	CLA	MG-NB	-2.34	2.01	2.05
24	6	612	CLA	CMC-C2C	-2.34	1.45	1.50
24	1	510	CLA	CMD-C2D	-2.34	1.45	1.50
24	B	606	CLA	C1B-C2B	2.34	1.48	1.43
34	BK	102	DGD	O2G-C2G	-2.34	1.40	1.46
23	Au	601	CHL	C3B-C4B	2.34	1.48	1.42
24	1	507	CLA	C3B-C4B	2.34	1.48	1.42
24	AA	303	CLA	MG-ND	-2.34	2.01	2.05
24	b	611	CLA	MG-NB	-2.34	2.01	2.05
23	BJ	609	CHL	C4B-NB	-2.34	1.34	1.37
23	BQ	608	CHL	C1B-NB	-2.34	1.34	1.37
25	G	615	LUT	C28-C29	-2.34	1.40	1.45
23	Ba	308	CHL	C3B-C4B	2.34	1.48	1.42
24	A	405	CLA	CMD-C2D	-2.34	1.45	1.50
24	c	507	CLA	MG-NB	-2.34	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	409	PHO	C3B-C2B	-2.34	1.37	1.40
23	AA	309	CHL	C3B-C4B	2.34	1.48	1.42
23	N	607	CHL	C4B-NB	-2.34	1.34	1.37
23	S	606	CHL	C1B-NB	-2.34	1.34	1.37
24	B	608	CLA	C1B-C2B	2.34	1.48	1.43
24	D	402	CLA	MG-NB	-2.34	2.01	2.05
24	b	616	CLA	MG-NB	-2.34	2.01	2.05
23	y	308	CHL	C3B-C4B	2.34	1.48	1.42
25	N	615	LUT	C12-C13	-2.34	1.40	1.45
23	Ba	306	CHL	C1B-C2B	2.34	1.48	1.43
34	BF	517	DGD	O1G-C1G	-2.34	1.39	1.45
24	S	602	CLA	MG-NB	-2.34	2.01	2.05
24	S	609	CLA	MG-NB	-2.33	2.01	2.05
24	Y	312	CLA	C1B-C2B	2.33	1.48	1.43
24	A2	603	CLA	CMB-C2B	-2.33	1.45	1.50
23	7	302	CHL	C4B-NB	-2.33	1.34	1.37
23	Y	310	CHL	MG-NA	-2.33	2.00	2.06
24	BB	312	CLA	CMB-C2B	-2.33	1.45	1.50
24	AA	311	CLA	MG-NB	-2.33	2.01	2.05
23	Au	606	CHL	C3B-C4B	2.33	1.48	1.42
23	Au	608	CHL	C3B-C4B	2.33	1.48	1.42
25	BV	614	LUT	C12-C13	-2.33	1.40	1.45
23	7	307	CHL	MG-NA	-2.33	2.00	2.06
24	B	614	CLA	MG-NB	-2.33	2.01	2.05
23	9	608	CHL	C1B-C2B	2.33	1.48	1.43
24	Y	303	CLA	C4B-NB	2.33	1.40	1.37
24	BU	609	CLA	C1B-NB	-2.33	1.34	1.37
24	C	513	CLA	MG-NB	-2.33	2.01	2.05
24	BB	312	CLA	MG-NB	-2.33	2.01	2.05
26	5	617	NEX	C32-C33	-2.33	1.40	1.45
23	AA	307	CHL	C1D-ND	-2.33	1.34	1.37
23	BV	605	CHL	C1B-NB	-2.33	1.34	1.37
34	A	402	DGD	O2G-C2G	-2.33	1.40	1.46
25	S	614	LUT	C28-C29	-2.33	1.40	1.45
24	c	508	CLA	CMD-C2D	-2.33	1.45	1.50
23	0	606	CHL	C4B-NB	-2.33	1.34	1.37
27	D	404	LHG	O7-C5	-2.33	1.40	1.46
24	9	604	CLA	CMD-C2D	-2.33	1.45	1.50
24	BE	612	CLA	MG-NB	-2.33	2.01	2.05
24	Ba	315	CLA	MG-NB	-2.33	2.01	2.05
23	N	609	CHL	C3B-C4B	2.33	1.48	1.42
25	n	615	LUT	C32-C33	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A2	617	NEX	C12-C13	-2.33	1.40	1.45
23	N	601	CHL	MG-NA	-2.33	2.00	2.06
23	BB	306	CHL	C3B-C4B	2.33	1.48	1.42
24	r	604	CLA	CMD-C2D	-2.33	1.45	1.50
24	r	610	CLA	CMD-C2D	-2.33	1.45	1.50
24	Au	603	CLA	MG-NB	-2.33	2.01	2.05
23	Y	310	CHL	C1D-ND	-2.33	1.34	1.37
24	C	505	CLA	MG-NB	-2.33	2.01	2.05
23	5	601	CHL	C1B-C2B	2.33	1.48	1.43
24	G	602	CLA	MG-NB	-2.33	2.01	2.05
25	A6	614	LUT	C28-C29	-2.33	1.40	1.45
23	BB	308	CHL	C1B-C2B	2.33	1.48	1.43
28	AA	301	XAT	C18-C5	2.33	1.55	1.51
23	A6	605	CHL	C1B-C2B	2.33	1.48	1.43
24	BE	616	CLA	MG-NB	-2.33	2.01	2.05
23	0	606	CHL	C1D-C2D	2.32	1.49	1.45
23	BU	605	CHL	C1D-C2D	2.32	1.49	1.45
23	Ba	302	CHL	C4C-C3C	2.32	1.49	1.45
23	N	605	CHL	C1D-ND	-2.32	1.34	1.37
26	5	617	NEX	C12-C13	-2.32	1.41	1.45
24	Au	613	CLA	MG-NB	-2.32	2.01	2.05
23	n	608	CHL	C1B-NB	-2.32	1.34	1.37
24	BB	315	CLA	C1B-C2B	2.32	1.48	1.43
24	1	509	CLA	C1B-C2B	2.32	1.48	1.43
24	6	610	CLA	MG-NB	-2.32	2.01	2.05
24	Y	312	CLA	MG-NB	-2.32	2.01	2.05
24	B	608	CLA	CMB-C2B	-2.32	1.45	1.50
38	R	408	PHO	C4D-ND	-2.32	1.35	1.38
24	c	512	CLA	C1B-C2B	2.32	1.48	1.43
24	BE	617	CLA	MG-NB	-2.32	2.01	2.05
24	0	613	CLA	C3B-C4B	2.32	1.48	1.42
23	AB	304	CHL	C3B-C4B	2.32	1.48	1.42
31	d	403	PL9	C52-C5	-2.32	1.45	1.50
23	Y	308	CHL	C1B-C2B	2.32	1.48	1.43
23	7	310	CHL	C3B-C4B	2.32	1.48	1.42
23	7	309	CHL	C4B-NB	-2.32	1.34	1.37
23	G	607	CHL	C1B-NB	-2.32	1.34	1.37
23	BB	309	CHL	C1D-ND	-2.32	1.34	1.37
23	N	606	CHL	MG-NA	-2.32	2.00	2.06
25	G	615	LUT	C32-C33	-2.32	1.41	1.45
24	8	308	CLA	C4B-NB	2.32	1.40	1.37
24	Au	602	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Az	101	SQD	C6-S	2.32	1.85	1.77
24	BU	612	CLA	C3B-C4B	2.32	1.48	1.42
23	AA	310	CHL	C3B-C4B	2.32	1.48	1.42
24	Y	303	CLA	C1B-C2B	2.32	1.48	1.43
23	Au	607	CHL	C1B-NB	-2.32	1.34	1.37
24	N	611	CLA	MG-NB	-2.32	2.01	2.05
24	1	512	CLA	C1B-C2B	2.32	1.48	1.43
24	Y	311	CLA	CMB-C2B	-2.32	1.45	1.50
23	g	601	CHL	C4C-C3C	2.32	1.49	1.45
24	BF	508	CLA	CMC-C2C	-2.32	1.45	1.50
24	AB	309	CLA	MG-NB	-2.32	2.01	2.05
24	N	602	CLA	CMB-C2B	-2.32	1.45	1.50
24	1	509	CLA	CMB-C2B	-2.32	1.45	1.50
24	BB	312	CLA	C1B-C2B	2.32	1.48	1.43
24	r	604	CLA	C1B-NB	-2.32	1.34	1.37
24	5	610	CLA	CHC-C1C	2.32	1.43	1.38
24	r	609	CLA	CMB-C2B	-2.32	1.45	1.50
23	7	302	CHL	C4C-C3C	2.32	1.49	1.45
25	Au	616	LUT	C12-C13	-2.32	1.41	1.45
24	8	302	CLA	CMD-C2D	-2.32	1.45	1.50
24	BB	313	CLA	C1B-C2B	2.31	1.48	1.43
23	0	608	CHL	C1D-ND	-2.31	1.34	1.37
23	AB	304	CHL	C4B-NB	-2.31	1.34	1.37
24	Y	304	CLA	CMB-C2B	-2.31	1.45	1.50
24	BF	513	CLA	CMD-C2D	-2.31	1.45	1.50
23	5	606	CHL	C1B-C2B	2.31	1.48	1.43
27	v	621	LHG	O7-C5	-2.31	1.40	1.46
23	BQ	608	CHL	C4B-NB	-2.31	1.34	1.37
25	Au	615	LUT	C32-C33	-2.31	1.41	1.45
24	6	611	CLA	C1B-C2B	2.31	1.48	1.43
24	0	611	CLA	C1B-C2B	2.31	1.48	1.43
23	A2	607	CHL	C3B-C4B	2.31	1.48	1.42
24	BU	609	CLA	CMB-C2B	-2.31	1.45	1.50
23	BQ	608	CHL	C4C-C3C	2.31	1.49	1.45
24	6	603	CLA	C1B-C2B	2.31	1.48	1.43
24	A2	611	CLA	MG-NB	-2.31	2.01	2.05
24	6	613	CLA	C3B-C4B	2.31	1.48	1.42
24	BF	514	CLA	C1B-C2B	2.31	1.48	1.43
24	0	611	CLA	CMB-C2B	-2.31	1.45	1.50
23	A2	606	CHL	MG-NA	-2.31	2.00	2.06
23	7	309	CHL	C3B-C4B	2.31	1.48	1.42
23	AA	308	CHL	C1B-C2B	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	601	CHL	MG-NA	-2.31	2.00	2.06
24	BF	510	CLA	CMB-C2B	-2.31	1.45	1.50
24	Au	602	CLA	MG-NB	-2.31	2.01	2.05
23	AA	308	CHL	C4B-NB	-2.31	1.34	1.37
24	AB	302	CLA	CMD-C2D	-2.31	1.45	1.50
23	y	309	CHL	C4C-C3C	2.31	1.49	1.45
23	n	605	CHL	C1B-NB	-2.31	1.34	1.37
24	G	611	CLA	CMD-C2D	-2.31	1.45	1.50
23	5	609	CHL	C1D-ND	-2.31	1.34	1.37
24	BV	604	CLA	CMC-C2C	-2.31	1.45	1.50
24	N	613	CLA	MG-NB	-2.31	2.01	2.05
24	c	510	CLA	CMD-C2D	-2.31	1.45	1.50
23	g	607	CHL	C1B-C2B	2.31	1.48	1.43
28	N	619	XAT	C18-C5	2.31	1.55	1.51
24	9	602	CLA	CMC-C2C	-2.31	1.45	1.50
23	AB	305	CHL	C1B-C2B	2.31	1.48	1.43
24	v	614	CLA	MG-NB	-2.30	2.01	2.05
25	6	616	LUT	C28-C29	-2.30	1.41	1.45
25	BJ	616	LUT	C32-C33	-2.30	1.41	1.45
26	S	616	NEX	C28-C29	-2.30	1.41	1.45
30	B	624	LMG	O7-C8	-2.30	1.40	1.46
24	b	612	CLA	MG-NB	-2.30	2.01	2.05
24	BF	505	CLA	MG-NB	-2.30	2.01	2.05
24	G	614	CLA	MG-NB	-2.30	2.01	2.05
24	B	603	CLA	MG-NB	-2.30	2.01	2.05
23	6	606	CHL	C4C-C3C	2.30	1.49	1.45
23	Y	309	CHL	C1D-ND	-2.30	1.35	1.37
23	n	606	CHL	C1B-NB	-2.30	1.35	1.37
23	BJ	607	CHL	C1B-C2B	2.30	1.48	1.43
24	BF	507	CLA	MG-NB	-2.30	2.01	2.05
24	BF	507	CLA	CMD-C2D	-2.30	1.45	1.50
24	A2	610	CLA	C1B-C2B	2.30	1.48	1.43
33	4	102	HEM	FE-NA	2.30	2.02	1.95
24	S	612	CLA	MG-NB	-2.30	2.01	2.05
24	B	602	CLA	MG-NB	-2.30	2.01	2.05
25	0	616	LUT	C32-C33	-2.30	1.41	1.45
24	c	509	CLA	CMB-C2B	-2.30	1.45	1.50
25	g	616	LUT	C32-C33	-2.30	1.41	1.45
30	BG	405	LMG	O7-C8	-2.30	1.40	1.46
24	BB	313	CLA	CMB-C2B	-2.30	1.45	1.50
23	g	609	CHL	C4B-NB	-2.30	1.35	1.37
34	h	102	DGD	O2G-C2G	-2.30	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	307	CHL	C3B-C4B	2.30	1.48	1.42
24	0	613	CLA	CMB-C2B	-2.30	1.45	1.50
24	BU	602	CLA	CMB-C2B	-2.30	1.45	1.50
24	a	406	CLA	MG-NB	-2.30	2.01	2.05
23	BV	601	CHL	C1B-C2B	2.30	1.48	1.43
24	G	602	CLA	CMC-C2C	-2.30	1.45	1.50
24	A6	612	CLA	MG-NB	-2.30	2.01	2.05
24	v	613	CLA	C1B-C2B	2.30	1.48	1.43
23	9	608	CHL	C3B-C4B	2.30	1.48	1.42
23	Ba	306	CHL	C1D-ND	-2.30	1.35	1.37
24	G	603	CLA	MG-NB	-2.30	2.01	2.05
23	BQ	606	CHL	MG-NA	-2.30	2.00	2.06
23	6	608	CHL	C1B-C2B	2.30	1.48	1.43
25	n	615	LUT	C28-C29	-2.30	1.41	1.45
23	Y	308	CHL	C4B-NB	-2.30	1.35	1.37
23	9	601	CHL	MG-NA	-2.30	2.00	2.06
24	C	502	CLA	C1B-C2B	2.30	1.48	1.43
24	G	602	CLA	CMB-C2B	-2.30	1.45	1.50
23	A2	609	CHL	C3B-C4B	2.29	1.48	1.42
24	Y	313	CLA	CMD-C2D	-2.29	1.45	1.50
23	g	605	CHL	C4C-C3C	2.29	1.49	1.45
24	B	607	CLA	MG-NB	-2.29	2.01	2.05
24	0	612	CLA	CMC-C2C	-2.29	1.45	1.50
23	Ba	309	CHL	C1B-NB	-2.29	1.35	1.37
24	1	508	CLA	C1B-C2B	2.29	1.48	1.43
24	BF	504	CLA	CMD-C2D	-2.29	1.45	1.50
23	Au	609	CHL	CBD-CGD	-2.29	1.49	1.51
23	AA	308	CHL	C3B-C4B	2.29	1.48	1.42
25	Au	616	LUT	C32-C33	-2.29	1.41	1.45
23	5	605	CHL	C1D-ND	-2.29	1.35	1.37
23	s	601	CHL	C1B-C2B	2.29	1.48	1.43
24	BB	303	CLA	CMD-C2D	-2.29	1.45	1.50
24	BB	312	CLA	CMD-C2D	-2.29	1.45	1.50
24	v	602	CLA	MG-NB	-2.29	2.01	2.05
24	BU	601	CLA	MG-ND	-2.29	2.01	2.05
24	8	309	CLA	MG-NB	-2.29	2.01	2.05
26	BQ	617	NEX	C28-C29	-2.29	1.41	1.45
34	C	517	DGD	O1G-C1G	-2.29	1.39	1.45
23	0	608	CHL	C1B-C2B	2.29	1.48	1.43
24	c	502	CLA	C1B-C2B	2.29	1.48	1.43
23	6	606	CHL	C4B-NB	-2.29	1.35	1.37
23	7	308	CHL	C1B-C2B	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	610	CLA	CMC-C2C	-2.29	1.45	1.50
24	BB	311	CLA	CMD-C2D	-2.29	1.45	1.50
24	BU	611	CLA	C1B-C2B	2.29	1.48	1.43
23	6	608	CHL	C1D-ND	-2.29	1.35	1.37
24	1	506	CLA	CMD-C2D	-2.29	1.45	1.50
24	1	509	CLA	C3B-C4B	2.29	1.48	1.42
24	5	603	CLA	C1B-C2B	2.29	1.48	1.43
23	y	302	CHL	C4C-C3C	2.29	1.49	1.45
24	5	602	CLA	CMC-C2C	-2.29	1.46	1.50
24	AB	308	CLA	CMD-C2D	-2.29	1.46	1.50
24	0	603	CLA	C1B-C2B	2.29	1.48	1.43
34	1	517	DGD	O1G-C1G	-2.29	1.39	1.45
26	n	617	NEX	C28-C29	-2.29	1.41	1.45
23	7	307	CHL	C4B-NB	-2.29	1.35	1.37
24	BB	304	CLA	CMD-C2D	-2.29	1.46	1.50
24	R	404	CLA	CMC-C2C	-2.29	1.46	1.50
24	BQ	604	CLA	MG-NB	-2.29	2.01	2.05
26	r	617	NEX	C32-C33	-2.28	1.41	1.45
24	9	612	CLA	C1B-C2B	2.28	1.48	1.43
24	BE	603	CLA	MG-NB	-2.28	2.01	2.05
23	7	308	CHL	MG-NA	-2.28	2.00	2.06
23	7	307	CHL	C4C-C3C	2.28	1.49	1.45
23	A6	606	CHL	C4C-C3C	2.28	1.49	1.45
23	0	606	CHL	C1D-ND	-2.28	1.35	1.37
25	BQ	615	LUT	C28-C29	-2.28	1.41	1.45
24	B	611	CLA	MG-NB	-2.28	2.01	2.05
24	v	612	CLA	MG-ND	-2.28	2.01	2.05
24	v	616	CLA	MG-NB	-2.28	2.01	2.05
24	s	609	CLA	CHC-C1C	2.28	1.43	1.38
23	Ba	307	CHL	MG-NA	-2.28	2.00	2.06
24	v	611	CLA	MG-NB	-2.28	2.01	2.05
23	Au	609	CHL	C4C-C3C	2.28	1.49	1.45
24	Au	604	CLA	CMB-C2B	-2.28	1.46	1.50
23	n	601	CHL	MG-NA	-2.28	2.00	2.06
28	g	619	XAT	C18-C5	2.28	1.55	1.51
23	6	607	CHL	C1D-ND	-2.28	1.35	1.37
24	v	611	CLA	CMD-C2D	-2.28	1.46	1.50
24	C	506	CLA	C1B-C2B	2.28	1.48	1.43
24	G	603	CLA	CMD-C2D	-2.28	1.46	1.50
23	BU	607	CHL	C4B-NB	-2.28	1.35	1.37
26	BB	320	NEX	C32-C33	-2.28	1.41	1.45
24	1	502	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	507	CLA	CMB-C2B	-2.28	1.46	1.50
24	y	311	CLA	CHC-C1C	2.28	1.43	1.38
24	0	602	CLA	CMB-C2B	-2.28	1.46	1.50
24	AB	303	CLA	CMD-C2D	-2.28	1.46	1.50
24	1	503	CLA	CMD-C2D	-2.28	1.46	1.50
24	G	604	CLA	MG-NB	-2.28	2.01	2.05
24	A6	608	CLA	MG-NB	-2.28	2.01	2.05
23	6	605	CHL	C1D-ND	-2.28	1.35	1.37
24	1	509	CLA	CMC-C2C	-2.28	1.46	1.50
23	N	606	CHL	C4B-NB	-2.28	1.35	1.37
23	Ba	307	CHL	C1B-NB	-2.28	1.35	1.37
24	v	612	CLA	CMC-C2C	-2.28	1.46	1.50
24	A2	610	CLA	CMB-C2B	-2.28	1.46	1.50
24	A2	613	CLA	MG-NB	-2.28	2.01	2.05
23	BB	307	CHL	C3B-C4B	2.28	1.48	1.42
24	7	313	CLA	CMD-C2D	-2.28	1.46	1.50
24	Y	311	CLA	CMC-C2C	-2.28	1.46	1.50
31	2	404	PL9	C26-C24	-2.28	1.46	1.51
23	n	609	CHL	C1B-NB	-2.28	1.35	1.37
23	s	605	CHL	C1B-NB	-2.28	1.35	1.37
23	Au	605	CHL	MG-NA	-2.28	2.00	2.06
24	A	407	CLA	CMD-C2D	-2.28	1.46	1.50
24	y	315	CLA	MG-NB	-2.28	2.01	2.05
24	6	610	CLA	CMD-C2D	-2.28	1.46	1.50
24	B	604	CLA	CMB-C2B	-2.28	1.46	1.50
24	y	312	CLA	CMB-C2B	-2.28	1.46	1.50
24	v	612	CLA	CMB-C2B	-2.28	1.46	1.50
23	A2	606	CHL	C4B-NB	-2.28	1.35	1.37
25	0	615	LUT	C32-C33	-2.27	1.41	1.45
23	7	309	CHL	MG-NA	-2.27	2.00	2.06
23	7	310	CHL	C1B-C2B	2.27	1.48	1.43
24	A2	603	CLA	C1B-C2B	2.27	1.48	1.43
24	v	603	CLA	MG-NB	-2.27	2.01	2.05
34	BK	102	DGD	CBB-CAB	-2.27	1.38	1.51
25	BQ	616	LUT	C28-C29	-2.27	1.41	1.45
24	C	510	CLA	CMD-C2D	-2.27	1.46	1.50
23	AB	306	CHL	CHB-C4A	-2.27	1.32	1.37
23	G	605	CHL	MG-NA	-2.27	2.00	2.06
24	1	512	CLA	CMD-C2D	-2.27	1.46	1.50
24	Au	604	CLA	MG-NB	-2.27	2.01	2.05
24	5	610	CLA	CMB-C2B	-2.27	1.46	1.50
31	2	404	PL9	C7-C8	-2.27	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	409	PHO	C4D-ND	-2.27	1.35	1.38
23	BH	601	CHL	C4C-C3C	2.27	1.49	1.45
34	a	401	DGD	O1G-C1G	-2.27	1.40	1.45
25	BV	614	LUT	C28-C29	-2.27	1.41	1.45
23	Y	308	CHL	C3B-C4B	2.27	1.48	1.42
38	BD	409	PHO	C3B-C2B	-2.27	1.37	1.40
24	0	610	CLA	CMD-C2D	-2.27	1.46	1.50
24	Ba	311	CLA	CHC-C1C	2.27	1.43	1.38
25	y	317	LUT	C28-C29	-2.27	1.41	1.45
23	Ba	309	CHL	C4C-C3C	2.27	1.49	1.45
24	BU	604	CLA	C1B-C2B	2.27	1.48	1.43
24	BU	614	CLA	MG-NB	-2.27	2.01	2.05
23	7	308	CHL	C3B-C4B	2.27	1.48	1.42
24	BF	502	CLA	C1B-C2B	2.27	1.48	1.43
24	G	604	CLA	CMB-C2B	-2.27	1.46	1.50
24	s	603	CLA	CHC-C1C	2.27	1.43	1.38
25	Ba	317	LUT	C28-C29	-2.27	1.41	1.45
24	BQ	602	CLA	CHC-C1C	2.27	1.43	1.38
24	BE	615	CLA	MG-NB	-2.27	2.01	2.05
23	BB	308	CHL	C3B-C4B	2.27	1.48	1.42
24	R	406	CLA	CMD-C2D	-2.27	1.46	1.50
24	BQ	610	CLA	CMC-C2C	-2.27	1.46	1.50
23	AA	306	CHL	C4B-NB	-2.27	1.35	1.37
24	BB	304	CLA	C1B-C2B	2.27	1.48	1.43
25	s	615	LUT	C28-C29	-2.27	1.41	1.45
24	r	601	CLA	C1B-C2B	2.27	1.48	1.43
28	Ba	301	XAT	C18-C5	2.27	1.55	1.51
23	n	601	CHL	C1B-NB	-2.27	1.35	1.37
23	s	605	CHL	C1D-ND	-2.27	1.35	1.37
23	5	606	CHL	MG-NA	-2.27	2.00	2.06
24	A2	611	CLA	CMD-C2D	-2.27	1.46	1.50
24	N	610	CLA	CHC-C1C	2.27	1.43	1.38
24	b	606	CLA	MG-NB	-2.27	2.01	2.05
24	r	614	CLA	MG-NB	-2.27	2.01	2.05
23	BQ	606	CHL	C1B-NB	-2.27	1.35	1.37
38	BD	409	PHO	C4D-ND	-2.27	1.35	1.38
24	Au	611	CLA	CMD-C2D	-2.27	1.46	1.50
23	BJ	605	CHL	C4C-C3C	2.27	1.48	1.45
24	A6	610	CLA	MG-NB	-2.27	2.01	2.05
24	BE	604	CLA	MG-NB	-2.27	2.01	2.05
23	8	307	CHL	C4C-C3C	2.27	1.48	1.45
23	AA	309	CHL	C4B-NB	-2.27	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	601	CHL	MG-NA	-2.27	2.00	2.06
23	y	307	CHL	MG-NA	-2.27	2.00	2.06
26	AA	319	NEX	C28-C29	-2.27	1.41	1.45
24	1	502	CLA	MG-NB	-2.26	2.01	2.05
23	y	306	CHL	C4C-C3C	2.26	1.48	1.45
24	c	513	CLA	CMD-C2D	-2.26	1.46	1.50
24	BF	504	CLA	CMB-C2B	-2.26	1.46	1.50
23	9	606	CHL	CHB-C4A	-2.26	1.32	1.37
23	7	307	CHL	C1D-ND	-2.26	1.35	1.37
24	A6	609	CLA	C1B-C2B	2.26	1.48	1.43
24	BE	606	CLA	MG-NB	-2.26	2.01	2.05
23	BB	310	CHL	MG-NA	-2.26	2.00	2.06
23	0	606	CHL	C1B-C2B	2.26	1.48	1.43
24	BE	610	CLA	MG-NB	-2.26	2.01	2.05
28	BQ	619	XAT	C18-C5	2.26	1.55	1.51
24	C	512	CLA	CMD-C2D	-2.26	1.46	1.50
23	S	601	CHL	C1D-ND	-2.26	1.35	1.37
23	Ba	302	CHL	C4B-NB	-2.26	1.35	1.37
24	N	602	CLA	CMD-C2D	-2.26	1.46	1.50
24	C	507	CLA	CMD-C2D	-2.26	1.46	1.50
23	Y	302	CHL	MG-NA	-2.26	2.00	2.06
24	BU	612	CLA	MG-ND	-2.26	2.01	2.05
23	S	607	CHL	C1B-NB	-2.26	1.35	1.37
26	7	319	NEX	C28-C29	-2.26	1.41	1.45
24	Ba	312	CLA	CMB-C2B	-2.26	1.46	1.50
24	1	511	CLA	CMD-C2D	-2.26	1.46	1.50
24	Y	312	CLA	CMB-C2B	-2.26	1.46	1.50
26	Au	617	NEX	C32-C33	-2.26	1.41	1.45
24	6	604	CLA	CMD-C2D	-2.26	1.46	1.50
24	S	609	CLA	C1B-C2B	2.26	1.48	1.43
24	8	308	CLA	MG-ND	-2.26	2.01	2.05
23	N	607	CHL	C1D-ND	-2.26	1.35	1.37
24	c	511	CLA	CMD-C2D	-2.26	1.46	1.50
23	Au	608	CHL	C1D-ND	-2.26	1.35	1.37
23	BU	606	CHL	C1D-ND	-2.26	1.35	1.37
24	y	303	CLA	CHC-C1C	2.26	1.43	1.38
24	C	508	CLA	CMB-C2B	-2.26	1.46	1.50
23	6	607	CHL	C3B-C4B	2.26	1.48	1.42
24	r	609	CLA	CMD-C2D	-2.26	1.46	1.50
24	BB	303	CLA	CMC-C2C	-2.26	1.46	1.50
24	1	508	CLA	CMD-C2D	-2.26	1.46	1.50
23	AB	304	CHL	C1D-ND	-2.26	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	MG-NB	-2.26	2.01	2.05
24	b	615	CLA	MG-NB	-2.26	2.01	2.05
24	r	602	CLA	C1B-C2B	2.26	1.48	1.43
24	BE	616	CLA	CMD-C2D	-2.26	1.46	1.50
24	7	311	CLA	MG-NB	-2.26	2.01	2.05
24	r	602	CLA	MG-ND	-2.26	2.01	2.05
24	B	611	CLA	CMB-C2B	-2.26	1.46	1.50
24	BB	315	CLA	CMB-C2B	-2.26	1.46	1.50
24	BE	612	CLA	CMB-C2B	-2.26	1.46	1.50
23	AA	308	CHL	MG-NA	-2.26	2.00	2.06
23	Ba	310	CHL	C1D-ND	-2.26	1.35	1.37
24	8	303	CLA	CMD-C2D	-2.26	1.46	1.50
24	c	510	CLA	CMB-C2B	-2.26	1.46	1.50
24	A2	603	CLA	CMD-C2D	-2.26	1.46	1.50
24	BF	503	CLA	CMD-C2D	-2.26	1.46	1.50
23	8	307	CHL	C1B-C2B	2.26	1.48	1.43
24	A2	612	CLA	CMD-C2D	-2.26	1.46	1.50
23	n	608	CHL	C4B-NB	-2.26	1.35	1.37
24	C	503	CLA	CMB-C2B	-2.26	1.46	1.50
24	5	604	CLA	CMD-C2D	-2.25	1.46	1.50
24	b	603	CLA	MG-NB	-2.25	2.01	2.05
24	Ba	303	CLA	CHC-C1C	2.25	1.43	1.38
23	9	601	CHL	C1B-C2B	2.25	1.48	1.43
23	5	601	CHL	MG-NA	-2.25	2.00	2.06
24	7	315	CLA	MG-NB	-2.25	2.01	2.05
30	d	405	LMG	O7-C8	-2.25	1.41	1.46
34	c	517	DGD	O1G-C1G	-2.25	1.40	1.45
24	BE	617	CLA	CMC-C2C	-2.25	1.46	1.50
24	1	502	CLA	CMB-C2B	-2.25	1.46	1.50
24	BD	405	CLA	CMD-C2D	-2.25	1.46	1.50
24	BF	511	CLA	CMC-C2C	-2.25	1.46	1.50
23	Ba	306	CHL	C4C-C3C	2.25	1.48	1.45
23	A6	601	CHL	MG-NA	-2.25	2.00	2.06
24	9	610	CLA	CMB-C2B	-2.25	1.46	1.50
25	n	616	LUT	C28-C29	-2.25	1.41	1.45
24	C	502	CLA	MG-NB	-2.25	2.01	2.05
25	BV	615	LUT	C28-C29	-2.25	1.41	1.45
24	c	508	CLA	CMC-C2C	-2.25	1.46	1.50
24	1	507	CLA	CMD-C2D	-2.25	1.46	1.50
23	y	302	CHL	C4B-NB	-2.25	1.35	1.37
23	r	613	CHL	C1B-C2B	2.25	1.48	1.43
24	BU	602	CLA	MG-ND	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	603	CLA	CMD-C2D	-2.25	1.46	1.50
24	b	605	CLA	CMB-C2B	-2.25	1.46	1.50
24	a	405	CLA	CMD-C2D	-2.25	1.46	1.50
23	n	607	CHL	C4C-C3C	2.25	1.48	1.45
24	y	313	CLA	MG-NB	-2.25	2.01	2.05
24	BE	605	CLA	CMB-C2B	-2.25	1.46	1.50
24	BV	610	CLA	MG-NB	-2.25	2.01	2.05
23	S	601	CHL	C1B-C2B	2.25	1.48	1.43
23	Y	302	CHL	C1B-C2B	2.25	1.48	1.43
23	n	606	CHL	C4C-C3C	2.25	1.48	1.45
24	B	605	CLA	CMD-C2D	-2.25	1.46	1.50
23	n	601	CHL	C4C-C3C	2.25	1.48	1.45
24	9	612	CLA	CMD-C2D	-2.25	1.46	1.50
24	v	605	CLA	CMD-C2D	-2.25	1.46	1.50
24	R	409	CLA	CMD-C2D	-2.25	1.46	1.50
24	BU	608	CLA	CMD-C2D	-2.25	1.46	1.50
23	9	606	CHL	C1B-C2B	2.25	1.48	1.43
23	AA	310	CHL	C1B-C2B	2.25	1.48	1.43
24	A	405	CLA	CMC-C2C	-2.25	1.46	1.50
24	A6	609	CLA	CMD-C2D	-2.25	1.46	1.50
24	BU	609	CLA	CMD-C2D	-2.25	1.46	1.50
23	BQ	605	CHL	C1B-NB	-2.25	1.35	1.37
24	Y	311	CLA	C4B-NB	2.25	1.40	1.37
24	1	511	CLA	CMB-C2B	-2.25	1.46	1.50
24	b	617	CLA	MG-NB	-2.25	2.01	2.05
24	s	608	CLA	MG-NB	-2.25	2.01	2.05
24	AA	315	CLA	MG-NB	-2.25	2.01	2.05
24	BV	608	CLA	MG-NB	-2.25	2.01	2.05
23	A6	606	CHL	C4B-NB	-2.24	1.35	1.37
24	Y	311	CLA	C1B-NB	-2.24	1.35	1.37
24	r	609	CLA	MG-ND	-2.24	2.01	2.05
24	C	509	CLA	CMB-C2B	-2.24	1.46	1.50
24	BV	612	CLA	MG-NB	-2.24	2.01	2.05
38	a	409	PHO	C3B-C2B	-2.24	1.37	1.40
24	6	610	CLA	CMB-C2B	-2.24	1.46	1.50
24	B	612	CLA	CMC-C2C	-2.24	1.46	1.50
24	b	612	CLA	CMD-C2D	-2.24	1.46	1.50
23	Au	608	CHL	CHB-C4A	-2.24	1.32	1.37
23	A6	601	CHL	C1D-ND	-2.24	1.35	1.37
23	BV	605	CHL	C1D-ND	-2.24	1.35	1.37
23	6	606	CHL	C1B-C2B	2.24	1.48	1.43
24	BF	506	CLA	CMB-C2B	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	616	LUT	C8-C9	-2.24	1.41	1.45
24	r	608	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	616	CLA	MG-NB	-2.24	2.01	2.05
24	Y	304	CLA	CMD-C2D	-2.24	1.46	1.50
24	Au	602	CLA	CMB-C2B	-2.24	1.46	1.50
23	BQ	601	CHL	MG-NA	-2.24	2.00	2.06
24	c	505	CLA	MG-NB	-2.24	2.01	2.05
24	v	610	CLA	CMD-C2D	-2.24	1.46	1.50
24	1	504	CLA	CMD-C2D	-2.24	1.46	1.50
23	Au	609	CHL	C1B-C2B	2.24	1.48	1.43
23	y	307	CHL	C1B-NB	-2.24	1.35	1.37
23	N	609	CHL	C1B-C2B	2.24	1.48	1.43
24	b	611	CLA	CMB-C2B	-2.24	1.46	1.50
23	y	308	CHL	C1B-NB	-2.24	1.35	1.37
24	B	611	CLA	CMC-C2C	-2.24	1.46	1.50
24	S	613	CLA	CMD-C2D	-2.24	1.46	1.50
24	b	617	CLA	CMC-C2C	-2.24	1.46	1.50
24	C	502	CLA	CMD-C2D	-2.24	1.46	1.50
25	S	615	LUT	C28-C29	-2.24	1.41	1.45
24	B	610	CLA	CMD-C2D	-2.24	1.46	1.50
24	N	603	CLA	CMB-C2B	-2.24	1.46	1.50
27	BQ	618	LHG	O7-C5	-2.24	1.41	1.46
24	9	610	CLA	CMD-C2D	-2.24	1.46	1.50
24	6	602	CLA	MG-ND	-2.24	2.01	2.05
24	s	612	CLA	MG-NB	-2.24	2.01	2.05
24	6	611	CLA	CMB-C2B	-2.24	1.46	1.50
23	N	609	CHL	MG-NA	-2.24	2.01	2.06
23	BV	607	CHL	C4B-NB	-2.24	1.35	1.37
23	Ba	302	CHL	C1D-ND	-2.24	1.35	1.37
24	r	602	CLA	C4B-NB	2.24	1.40	1.37
24	8	308	CLA	CMA-C3A	-2.24	1.48	1.53
27	Ba	319	LHG	O7-C5	-2.24	1.41	1.46
24	B	606	CLA	CMD-C2D	-2.24	1.46	1.50
24	r	603	CLA	CMB-C2B	-2.24	1.46	1.50
24	BV	613	CLA	CMB-C2B	-2.24	1.46	1.50
24	BU	609	CLA	MG-ND	-2.24	2.01	2.05
23	Ba	309	CHL	C4B-NB	-2.24	1.35	1.37
23	BU	607	CHL	C1D-ND	-2.24	1.35	1.37
24	A6	602	CLA	CMB-C2B	-2.24	1.46	1.50
24	c	510	CLA	C3B-C4B	2.24	1.48	1.42
24	Y	312	CLA	CMD-C2D	-2.24	1.46	1.50
23	AA	309	CHL	MG-NA	-2.24	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	CMD-C2D	-2.24	1.46	1.50
23	BQ	606	CHL	C4C-C3C	2.23	1.48	1.45
24	r	612	CLA	MG-ND	-2.23	2.01	2.05
29	K	101	BCR	C33-C5	-2.23	1.47	1.50
24	Au	612	CLA	CMC-C2C	-2.23	1.46	1.50
23	7	308	CHL	CHB-C4A	-2.23	1.32	1.37
23	y	310	CHL	C4B-NB	-2.23	1.35	1.37
24	r	611	CLA	CMB-C2B	-2.23	1.46	1.50
24	BD	407	CLA	CMD-C2D	-2.23	1.46	1.50
23	N	606	CHL	C1B-C2B	2.23	1.48	1.43
23	A6	601	CHL	C1B-C2B	2.23	1.48	1.43
24	BF	513	CLA	CMB-C2B	-2.23	1.46	1.50
23	y	310	CHL	C1D-ND	-2.23	1.35	1.37
24	7	303	CLA	MG-ND	-2.23	2.01	2.05
23	S	606	CHL	C4C-C3C	2.23	1.48	1.45
24	C	507	CLA	CMB-C2B	-2.23	1.46	1.50
24	r	602	CLA	CMB-C2B	-2.23	1.46	1.50
24	n	604	CLA	MG-NB	-2.23	2.01	2.05
24	S	610	CLA	MG-NB	-2.23	2.01	2.05
28	y	301	XAT	C18-C5	2.23	1.55	1.51
23	BQ	601	CHL	C4C-C3C	2.23	1.48	1.45
24	BB	314	CLA	CMC-C2C	-2.23	1.46	1.50
25	9	615	LUT	C28-C29	-2.23	1.41	1.45
24	v	607	CLA	CMD-C2D	-2.23	1.46	1.50
24	y	312	CLA	MG-NB	-2.23	2.01	2.05
24	BU	610	CLA	C1B-NB	-2.23	1.35	1.37
24	A2	602	CLA	CMD-C2D	-2.23	1.46	1.50
24	R	404	CLA	CMB-C2B	-2.23	1.46	1.50
24	BF	502	CLA	CMB-C2B	-2.23	1.46	1.50
24	BU	602	CLA	C1B-C2B	2.23	1.48	1.43
23	r	607	CHL	C1D-ND	-2.23	1.35	1.37
23	BQ	601	CHL	C1B-NB	-2.23	1.35	1.37
24	BF	508	CLA	C1B-NB	-2.23	1.35	1.37
24	BF	502	CLA	MG-NB	-2.23	2.01	2.05
24	1	506	CLA	C1B-C2B	2.23	1.48	1.43
24	A6	613	CLA	CMD-C2D	-2.23	1.46	1.50
24	b	602	CLA	MG-NB	-2.23	2.01	2.05
23	6	606	CHL	CHB-C4A	-2.23	1.32	1.37
23	AA	307	CHL	C4C-C3C	2.23	1.48	1.45
24	BD	406	CLA	CMD-C2D	-2.23	1.46	1.50
24	BF	508	CLA	CMB-C2B	-2.23	1.46	1.50
23	r	607	CHL	C1B-C2B	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BV	603	CLA	CHC-C1C	2.23	1.43	1.38
26	G	617	NEX	C32-C33	-2.23	1.41	1.45
24	BU	602	CLA	C4B-NB	2.23	1.40	1.37
24	N	610	CLA	CMB-C2B	-2.23	1.46	1.50
28	A2	619	XAT	C18-C5	2.23	1.55	1.51
24	5	614	CLA	MG-NB	-2.23	2.01	2.05
23	Ba	308	CHL	C4B-NB	-2.23	1.35	1.37
24	Ba	312	CLA	MG-NB	-2.23	2.01	2.05
31	BG	403	PL9	C26-C24	-2.23	1.46	1.51
24	c	507	CLA	C1B-C2B	2.23	1.48	1.43
24	C	503	CLA	CMD-C2D	-2.23	1.46	1.50
24	BE	615	CLA	CMD-C2D	-2.23	1.46	1.50
24	BD	406	CLA	CMB-C2B	-2.23	1.46	1.50
32	R	411	SQD	O9-S	2.23	1.51	1.45
24	AA	311	CLA	CHC-C1C	2.23	1.43	1.38
24	Aw	102	CLA	C1B-C2B	2.23	1.48	1.43
24	9	611	CLA	MG-NB	-2.23	2.01	2.05
23	7	307	CHL	C3B-C4B	2.23	1.48	1.42
24	7	313	CLA	MG-NB	-2.23	2.01	2.05
23	7	310	CHL	C4C-C3C	2.22	1.48	1.45
29	AB	313	BCR	C33-C5	-2.22	1.47	1.50
23	A2	607	CHL	MG-NA	-2.22	2.01	2.06
24	1	507	CLA	CMC-C2C	-2.22	1.46	1.50
23	y	306	CHL	C1D-ND	-2.22	1.35	1.37
34	1	516	DGD	O2G-C2G	-2.22	1.41	1.46
24	c	508	CLA	C3B-C4B	2.22	1.48	1.42
23	y	309	CHL	C1D-ND	-2.22	1.35	1.37
24	C	511	CLA	C1B-NB	-2.22	1.35	1.37
23	N	607	CHL	C1B-C2B	2.22	1.48	1.43
24	S	608	CLA	MG-NB	-2.22	2.01	2.05
24	b	614	CLA	CMB-C2B	-2.22	1.46	1.50
24	y	314	CLA	CMB-C2B	-2.22	1.46	1.50
34	BF	518	DGD	O1G-C1G	-2.22	1.40	1.45
23	BB	302	CHL	CHB-C4A	-2.22	1.32	1.37
38	BD	408	PHO	C3B-CAB	-2.22	1.43	1.47
24	v	606	CLA	CMD-C2D	-2.22	1.46	1.50
24	A2	613	CLA	CMB-C2B	-2.22	1.46	1.50
24	BF	511	CLA	CMB-C2B	-2.22	1.46	1.50
25	5	616	LUT	C32-C33	-2.22	1.41	1.45
24	BB	303	CLA	C1B-C2B	2.22	1.48	1.43
23	r	606	CHL	C1D-ND	-2.22	1.35	1.37
23	A2	605	CHL	MG-NA	-2.22	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	MG-NB	-2.22	2.01	2.05
24	s	611	CLA	MG-NB	-2.22	2.01	2.05
24	b	606	CLA	CMD-C2D	-2.22	1.46	1.50
24	n	602	CLA	CHC-C1C	2.22	1.43	1.38
24	BU	601	CLA	CMB-C2B	-2.22	1.46	1.50
23	BV	601	CHL	MG-NA	-2.22	2.01	2.06
30	v	623	LMG	O7-C8	-2.22	1.41	1.46
24	BB	311	CLA	C4B-NB	2.22	1.40	1.37
24	N	611	CLA	CMD-C2D	-2.22	1.46	1.50
24	BE	611	CLA	CMB-C2B	-2.22	1.46	1.50
24	Y	315	CLA	CMB-C2B	-2.22	1.46	1.50
24	v	613	CLA	CMB-C2B	-2.22	1.46	1.50
24	1	510	CLA	CMC-C2C	-2.22	1.46	1.50
24	BF	514	CLA	CMB-C2B	-2.22	1.46	1.50
23	5	606	CHL	CHB-C4A	-2.22	1.32	1.37
28	BJ	619	XAT	C18-C5	2.22	1.55	1.51
23	N	607	CHL	MG-NA	-2.22	2.01	2.06
24	6	603	CLA	CMB-C2B	-2.22	1.46	1.50
24	A	410	CLA	CMD-C2D	-2.22	1.46	1.50
24	BE	606	CLA	CMD-C2D	-2.22	1.46	1.50
24	y	311	CLA	MG-NB	-2.22	2.01	2.05
24	A6	612	CLA	CMB-C2B	-2.22	1.46	1.50
23	s	607	CHL	C4B-NB	-2.22	1.35	1.37
23	AB	307	CHL	C1B-C2B	2.22	1.48	1.43
24	AA	311	CLA	CBD-CGD	-2.22	1.49	1.51
24	B	612	CLA	CMB-C2B	-2.22	1.46	1.50
24	A	410	CLA	CMB-C2B	-2.22	1.46	1.50
24	a	406	CLA	CMD-C2D	-2.22	1.46	1.50
24	A6	611	CLA	CMD-C2D	-2.22	1.46	1.50
23	A2	607	CHL	C1B-C2B	2.22	1.48	1.43
28	n	619	XAT	C18-C5	2.22	1.55	1.51
24	0	610	CLA	CMB-C2B	-2.22	1.46	1.50
23	Au	609	CHL	C3B-C4B	2.22	1.48	1.42
23	BU	607	CHL	CHB-C4A	-2.22	1.32	1.37
24	BJ	610	CLA	CHC-C1C	2.22	1.43	1.38
25	A6	615	LUT	C28-C29	-2.22	1.41	1.45
24	0	603	CLA	MG-ND	-2.21	2.01	2.05
24	Y	311	CLA	CMD-C2D	-2.21	1.46	1.50
38	a	409	PHO	C4D-ND	-2.21	1.35	1.38
23	BB	302	CHL	C1B-C2B	2.21	1.48	1.43
23	S	601	CHL	C4C-C3C	2.21	1.48	1.45
23	0	606	CHL	CHB-C4A	-2.21	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	609	CLA	CHC-C1C	2.21	1.43	1.38
24	b	616	CLA	CMD-C2D	-2.21	1.46	1.50
24	9	612	CLA	CMB-C2B	-2.21	1.46	1.50
24	BV	612	CLA	CMB-C2B	-2.21	1.46	1.50
24	0	602	CLA	C4B-NB	2.21	1.40	1.37
24	Au	602	CLA	CMC-C2C	-2.21	1.46	1.50
23	AA	307	CHL	C3B-C4B	2.21	1.48	1.42
24	BV	609	CLA	CHC-C1C	2.21	1.43	1.38
24	2	402	CLA	CMC-C2C	-2.21	1.46	1.50
24	1	512	CLA	CMB-C2B	-2.21	1.46	1.50
27	BE	622	LHG	O7-C5	-2.21	1.41	1.46
23	AA	308	CHL	CHB-C4A	-2.21	1.32	1.37
23	N	605	CHL	MG-NA	-2.21	2.01	2.06
24	N	604	CLA	CMB-C2B	-2.21	1.46	1.50
24	r	610	CLA	CMC-C2C	-2.21	1.46	1.50
23	G	605	CHL	C4C-C3C	2.21	1.48	1.45
24	A6	603	CLA	MG-NB	-2.21	2.01	2.05
24	B	611	CLA	CMD-C2D	-2.21	1.46	1.50
24	B	613	CLA	CMD-C2D	-2.21	1.46	1.50
24	c	514	CLA	CMB-C2B	-2.21	1.46	1.50
24	BE	614	CLA	CMB-C2B	-2.21	1.46	1.50
24	N	612	CLA	CMD-C2D	-2.21	1.46	1.50
24	0	603	CLA	CMB-C2B	-2.21	1.46	1.50
24	BU	601	CLA	CMD-C2D	-2.21	1.46	1.50
24	1	502	CLA	C1B-C2B	2.21	1.48	1.43
24	C	508	CLA	CMD-C2D	-2.21	1.46	1.50
24	BU	611	CLA	CMB-C2B	-2.21	1.46	1.50
23	BQ	607	CHL	C1B-NB	-2.21	1.35	1.37
24	9	602	CLA	C1B-C2B	2.21	1.48	1.43
24	G	612	CLA	CMC-C2C	-2.21	1.46	1.50
24	A2	612	CLA	CMB-C2B	-2.21	1.46	1.50
24	A6	604	CLA	CMB-C2B	-2.21	1.46	1.50
24	BU	602	CLA	CMD-C2D	-2.21	1.46	1.50
24	0	602	CLA	MG-ND	-2.21	2.01	2.05
23	BU	607	CHL	C1B-C2B	2.21	1.48	1.43
27	n	618	LHG	O7-C5	-2.21	1.41	1.46
34	C	516	DGD	O2G-C2G	-2.21	1.41	1.46
24	A2	604	CLA	CMB-C2B	-2.21	1.46	1.50
32	BD	412	SQD	O9-S	2.21	1.51	1.45
24	C	502	CLA	CMB-C2B	-2.21	1.46	1.50
24	v	613	CLA	CMD-C2D	-2.21	1.46	1.50
24	BB	313	CLA	MG-ND	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BE	602	CLA	MG-NB	-2.21	2.01	2.05
23	5	601	CHL	C1D-ND	-2.21	1.35	1.37
23	G	607	CHL	C4B-NB	-2.21	1.35	1.37
23	S	605	CHL	C1B-NB	-2.21	1.35	1.37
23	BV	607	CHL	C1B-NB	-2.21	1.35	1.37
24	c	508	CLA	C1B-NB	-2.21	1.35	1.37
24	7	314	CLA	CMD-C2D	-2.21	1.46	1.50
24	N	604	CLA	CMD-C2D	-2.21	1.46	1.50
24	Y	303	CLA	CMD-C2D	-2.21	1.46	1.50
24	c	511	CLA	CMB-C2B	-2.21	1.46	1.50
24	5	602	CLA	CHC-C1C	2.21	1.43	1.38
26	n	617	NEX	C12-C13	-2.21	1.41	1.45
23	A2	605	CHL	C4B-NB	-2.21	1.35	1.37
24	6	602	CLA	C1B-NB	-2.21	1.35	1.37
24	1	509	CLA	CMD-C2D	-2.21	1.46	1.50
27	b	622	LHG	O7-C5	-2.21	1.41	1.46
23	Au	606	CHL	C4B-NB	-2.21	1.35	1.37
38	A	408	PHO	C3B-CAB	-2.21	1.43	1.47
32	BG	406	SQD	O9-S	2.20	1.51	1.45
24	b	610	CLA	MG-NB	-2.20	2.01	2.05
24	D	401	CLA	CMC-C2C	-2.20	1.46	1.50
26	y	318	NEX	C28-C29	-2.20	1.41	1.45
24	g	602	CLA	MG-NB	-2.20	2.01	2.05
24	c	511	CLA	CMC-C2C	-2.20	1.46	1.50
24	9	604	CLA	CMB-C2B	-2.20	1.46	1.50
24	BU	608	CLA	CMB-C2B	-2.20	1.46	1.50
32	A	413	SQD	O9-S	2.20	1.51	1.45
24	7	315	CLA	CHC-C1C	2.20	1.43	1.38
24	g	610	CLA	CHC-C1C	2.20	1.43	1.38
23	8	306	CHL	CHB-C4A	-2.20	1.32	1.37
24	5	604	CLA	CMB-C2B	-2.20	1.46	1.50
24	BD	410	CLA	CMB-C2B	-2.20	1.46	1.50
23	s	601	CHL	MG-NA	-2.20	2.01	2.06
24	C	509	CLA	CMC-C2C	-2.20	1.46	1.50
24	v	614	CLA	CMD-C2D	-2.20	1.46	1.50
24	Ba	311	CLA	MG-NB	-2.20	2.01	2.05
34	BD	401	DGD	O1G-C1G	-2.20	1.40	1.45
24	s	610	CLA	MG-NB	-2.20	2.01	2.05
26	Ba	318	NEX	C28-C29	-2.20	1.41	1.45
24	BF	502	CLA	CMC-C2C	-2.20	1.46	1.50
24	c	506	CLA	CMB-C2B	-2.20	1.46	1.50
24	r	602	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	611	CLA	CMC-C2C	-2.20	1.46	1.50
24	1	512	CLA	CMC-C2C	-2.20	1.46	1.50
23	Au	601	CHL	C4B-NB	-2.20	1.35	1.37
23	Ba	308	CHL	C1B-NB	-2.20	1.35	1.37
24	8	301	CLA	C1B-NB	-2.20	1.35	1.37
24	BF	510	CLA	C3B-C4B	2.20	1.47	1.42
24	a	410	CLA	CMB-C2B	-2.20	1.46	1.50
27	B	621	LHG	O7-C5	-2.20	1.41	1.46
24	7	311	CLA	CMC-C2C	-2.20	1.46	1.50
24	A	405	CLA	CMB-C2B	-2.20	1.46	1.50
24	a	406	CLA	CMB-C2B	-2.20	1.46	1.50
24	BU	608	CLA	CMC-C2C	-2.20	1.46	1.50
23	Y	310	CHL	C1B-C2B	2.20	1.48	1.43
23	0	607	CHL	C3B-C4B	2.20	1.47	1.42
24	1	505	CLA	CMD-C2D	-2.20	1.46	1.50
24	9	602	CLA	CHC-C1C	2.20	1.43	1.38
24	c	513	CLA	CMB-C2B	-2.20	1.46	1.50
24	Ba	313	CLA	MG-NB	-2.20	2.01	2.05
24	S	611	CLA	CMD-C2D	-2.20	1.46	1.50
23	BQ	605	CHL	C4C-C3C	2.20	1.48	1.45
32	d	406	SQD	O9-S	2.20	1.51	1.45
24	C	506	CLA	CMD-C2D	-2.20	1.46	1.50
24	C	511	CLA	CMB-C2B	-2.20	1.46	1.50
24	9	603	CLA	CMC-C2C	-2.20	1.46	1.50
23	0	606	CHL	C4C-C3C	2.20	1.48	1.45
23	A6	601	CHL	C4C-C3C	2.20	1.48	1.45
24	B	612	CLA	MG-ND	-2.20	2.01	2.05
24	S	612	CLA	CMB-C2B	-2.20	1.46	1.50
24	A	406	CLA	CMB-C2B	-2.20	1.46	1.50
24	R	409	CLA	CMB-C2B	-2.20	1.46	1.50
24	5	610	CLA	CMD-C2D	-2.19	1.46	1.50
24	5	611	CLA	MG-NB	-2.19	2.01	2.05
31	D	403	PL9	C20-C19	-2.19	1.45	1.50
23	BB	302	CHL	C4B-NB	-2.19	1.35	1.37
26	y	318	NEX	C32-C33	-2.19	1.41	1.45
23	G	608	CHL	CHB-C4A	-2.19	1.32	1.37
24	Y	313	CLA	CMB-C2B	-2.19	1.46	1.50
24	S	604	CLA	CMD-C2D	-2.19	1.46	1.50
24	b	613	CLA	CMD-C2D	-2.19	1.46	1.50
24	c	510	CLA	CMC-C2C	-2.19	1.46	1.50
24	BV	611	CLA	MG-NB	-2.19	2.01	2.05
24	N	603	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	604	CLA	CMD-C2D	-2.19	1.46	1.50
24	BE	603	CLA	CMD-C2D	-2.19	1.46	1.50
24	BU	611	CLA	MG-ND	-2.19	2.01	2.05
24	BB	314	CLA	CMB-C2B	-2.19	1.46	1.50
24	BJ	602	CLA	MG-NB	-2.19	2.01	2.05
23	7	302	CHL	C1B-C2B	2.19	1.48	1.43
23	AA	309	CHL	C1B-NB	-2.19	1.35	1.37
24	5	612	CLA	CMB-C2B	-2.19	1.46	1.50
24	r	608	CLA	CMB-C2B	-2.19	1.46	1.50
24	A6	611	CLA	CMB-C2B	-2.19	1.46	1.50
24	Ba	314	CLA	CMB-C2B	-2.19	1.46	1.50
24	BU	612	CLA	CMD-C2D	-2.19	1.46	1.50
24	8	310	CLA	CMB-C2B	-2.19	1.46	1.50
24	A2	611	CLA	CMB-C2B	-2.19	1.46	1.50
24	Ba	314	CLA	MG-NB	-2.19	2.01	2.05
27	y	319	LHG	O7-C5	-2.19	1.41	1.46
24	a	405	CLA	CMB-C2B	-2.19	1.46	1.50
24	9	613	CLA	CMC-C2C	-2.19	1.46	1.50
24	1	503	CLA	CMC-C2C	-2.19	1.46	1.50
31	D	403	PL9	C26-C24	-2.19	1.46	1.51
23	9	607	CHL	CHB-C4A	-2.19	1.32	1.37
24	1	510	CLA	CMB-C2B	-2.19	1.46	1.50
23	6	605	CHL	C4C-C3C	2.19	1.48	1.45
24	9	610	CLA	CHC-C1C	2.19	1.43	1.38
24	7	304	CLA	CMB-C2B	-2.19	1.46	1.50
24	BB	305	CLA	CMC-C2C	-2.19	1.46	1.50
23	s	601	CHL	C4C-C3C	2.19	1.48	1.45
24	A2	603	CLA	CMC-C2C	-2.19	1.46	1.50
24	9	604	CLA	C1B-NB	-2.19	1.35	1.37
24	B	613	CLA	CMB-C2B	-2.19	1.46	1.50
24	BB	315	CLA	CMD-C2D	-2.19	1.46	1.50
24	BU	603	CLA	CMB-C2B	-2.19	1.46	1.50
24	BU	604	CLA	CMB-C2B	-2.19	1.46	1.50
32	L	101	SQD	O9-S	2.19	1.51	1.45
23	S	606	CHL	MG-NA	-2.19	2.01	2.06
25	g	616	LUT	C28-C29	-2.19	1.41	1.45
23	A6	606	CHL	C1D-ND	-2.19	1.35	1.37
23	BU	613	CHL	C1B-C2B	2.19	1.48	1.43
24	C	505	CLA	CMD-C2D	-2.19	1.46	1.50
24	v	609	CLA	CMD-C2D	-2.19	1.46	1.50
24	A6	604	CLA	CMD-C2D	-2.19	1.46	1.50
24	Au	602	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	613	CLA	MG-ND	-2.19	2.01	2.05
23	0	605	CHL	C4B-NB	-2.19	1.35	1.37
23	n	605	CHL	C4C-C3C	2.19	1.48	1.45
24	Au	603	CLA	CMB-C2B	-2.19	1.46	1.50
23	6	607	CHL	C1B-C2B	2.19	1.48	1.43
23	8	306	CHL	C4C-C3C	2.19	1.48	1.45
23	e	601	CHL	C4C-C3C	2.19	1.48	1.45
26	n	617	NEX	C32-C33	-2.19	1.41	1.45
24	5	603	CLA	CMC-C2C	-2.19	1.46	1.50
24	N	613	CLA	CMB-C2B	-2.19	1.46	1.50
24	Ba	313	CLA	CMB-C2B	-2.19	1.46	1.50
24	BF	505	CLA	CHC-C1C	2.19	1.43	1.38
24	6	613	CLA	MG-ND	-2.19	2.01	2.05
24	S	611	CLA	CMC-C2C	-2.19	1.46	1.50
23	0	607	CHL	C1B-C2B	2.19	1.48	1.43
24	c	502	CLA	MG-NB	-2.19	2.01	2.05
23	5	607	CHL	CHB-C4A	-2.19	1.32	1.37
28	AA	318	XAT	C18-C5	2.18	1.55	1.51
24	y	305	CLA	MG-NB	-2.18	2.01	2.05
26	s	616	NEX	C12-C13	-2.18	1.41	1.45
26	BV	616	NEX	C28-C29	-2.18	1.41	1.45
24	1	508	CLA	CMC-C2C	-2.18	1.46	1.50
23	AA	310	CHL	C4C-C3C	2.18	1.48	1.45
24	n	613	CLA	MG-NB	-2.18	2.01	2.05
25	9	615	LUT	C32-C33	-2.18	1.41	1.45
24	v	605	CLA	CMB-C2B	-2.18	1.46	1.50
23	n	607	CHL	C1B-NB	-2.18	1.35	1.37
24	BQ	613	CLA	MG-NB	-2.18	2.01	2.05
24	c	504	CLA	CMD-C2D	-2.18	1.46	1.50
24	BE	611	CLA	CMD-C2D	-2.18	1.46	1.50
23	Y	307	CHL	CHB-C4A	-2.18	1.32	1.37
23	A2	606	CHL	C1B-C2B	2.18	1.48	1.43
24	Ba	305	CLA	MG-NB	-2.18	2.01	2.05
24	B	616	CLA	CMB-C2B	-2.18	1.46	1.50
24	c	514	CLA	CMD-C2D	-2.18	1.46	1.50
24	AA	313	CLA	MG-NB	-2.18	2.01	2.05
24	B	614	CLA	CMD-C2D	-2.18	1.46	1.50
23	BQ	607	CHL	C4C-C3C	2.18	1.48	1.45
24	S	602	CLA	CMB-C2B	-2.18	1.46	1.50
23	6	605	CHL	C4B-NB	-2.18	1.35	1.37
23	g	601	CHL	C1B-NB	-2.18	1.35	1.37
24	BE	606	CLA	CHC-C1C	2.18	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	606	CHL	C1B-C2B	2.18	1.48	1.43
26	A2	617	NEX	C1-C6	-2.18	1.50	1.54
24	5	612	CLA	CMD-C2D	-2.18	1.46	1.50
24	AA	314	CLA	CMD-C2D	-2.18	1.46	1.50
24	1	513	CLA	CMB-C2B	-2.18	1.46	1.50
24	v	603	CLA	CHC-C1C	2.18	1.43	1.38
23	N	605	CHL	C3B-C4B	2.18	1.47	1.42
24	A6	602	CLA	CMD-C2D	-2.18	1.46	1.50
24	a	407	CLA	CMD-C2D	-2.18	1.46	1.50
24	B	609	CLA	MG-ND	-2.18	2.01	2.05
24	BF	503	CLA	MG-ND	-2.18	2.01	2.05
38	a	408	PHO	C3B-CAB	-2.18	1.43	1.47
24	A2	610	CLA	CHC-C1C	2.18	1.43	1.38
24	9	614	CLA	MG-NB	-2.18	2.01	2.05
24	BU	603	CLA	MG-ND	-2.18	2.01	2.05
23	N	605	CHL	C4B-NB	-2.18	1.35	1.37
26	A6	616	NEX	C12-C13	-2.18	1.41	1.45
23	A2	605	CHL	C3B-C4B	2.18	1.47	1.42
24	r	612	CLA	CMB-C2B	-2.18	1.46	1.50
23	8	305	CHL	CHB-C4A	-2.18	1.32	1.37
24	r	601	CLA	MG-ND	-2.18	2.01	2.05
26	Au	617	NEX	C28-C29	-2.18	1.41	1.45
26	Ba	318	NEX	C32-C33	-2.18	1.41	1.45
32	BO	101	SQD	O7-S	2.18	1.51	1.45
38	R	407	PHO	C3B-CAB	-2.18	1.43	1.47
23	Y	302	CHL	C1D-ND	-2.18	1.35	1.37
24	a	410	CLA	CMD-C2D	-2.18	1.46	1.50
24	BB	313	CLA	CMC-C2C	-2.18	1.46	1.50
23	G	609	CHL	CBD-CGD	-2.18	1.49	1.51
24	BB	315	CLA	MG-ND	-2.18	2.01	2.05
24	C	504	CLA	CMD-C2D	-2.18	1.46	1.50
24	r	608	CLA	CMC-C2C	-2.18	1.46	1.50
23	s	601	CHL	C1D-ND	-2.18	1.35	1.37
24	G	610	CLA	CMB-C2B	-2.18	1.46	1.50
25	5	616	LUT	C12-C13	-2.18	1.41	1.45
25	BJ	616	LUT	C28-C29	-2.18	1.41	1.45
24	1	505	CLA	CMB-C2B	-2.18	1.46	1.50
24	N	613	CLA	CMD-C2D	-2.18	1.46	1.50
24	S	611	CLA	CMB-C2B	-2.18	1.46	1.50
24	c	502	CLA	CMB-C2B	-2.18	1.46	1.50
24	BU	612	CLA	CMB-C2B	-2.18	1.46	1.50
32	a	412	SQD	O9-S	2.18	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	v	606	CLA	MG-NB	-2.18	2.01	2.05
24	c	504	CLA	CMB-C2B	-2.18	1.46	1.50
24	BQ	604	CLA	CMB-C2B	-2.18	1.46	1.50
23	G	606	CHL	C4B-NB	-2.18	1.35	1.37
24	c	505	CLA	CHC-C1C	2.17	1.42	1.38
24	BJ	611	CLA	CHC-C1C	2.17	1.42	1.38
24	0	614	CLA	MG-ND	-2.17	2.01	2.05
24	s	612	CLA	CMB-C2B	-2.17	1.46	1.50
24	C	512	CLA	CMB-C2B	-2.17	1.46	1.50
23	7	306	CHL	C4B-NB	-2.17	1.35	1.37
24	BD	407	CLA	CMB-C2B	-2.17	1.46	1.50
25	9	616	LUT	C12-C13	-2.17	1.41	1.45
23	BB	308	CHL	MG-NA	-2.17	2.01	2.06
24	v	616	CLA	CMB-C2B	-2.17	1.46	1.50
26	AA	319	NEX	C32-C33	-2.17	1.41	1.45
24	c	508	CLA	CMB-C2B	-2.17	1.46	1.50
24	BG	401	CLA	CMB-C2B	-2.17	1.46	1.50
23	r	607	CHL	C4B-NB	-2.17	1.35	1.37
30	c	518	LMG	O7-C8	-2.17	1.41	1.46
24	Y	314	CLA	CMB-C2B	-2.17	1.46	1.50
24	AB	310	CLA	CMB-C2B	-2.17	1.46	1.50
24	BU	601	CLA	CMC-C2C	-2.17	1.46	1.50
24	B	615	CLA	CMD-C2D	-2.17	1.46	1.50
24	A2	613	CLA	CMD-C2D	-2.17	1.46	1.50
24	A6	611	CLA	CMC-C2C	-2.17	1.46	1.50
23	BB	302	CHL	MG-NA	-2.17	2.01	2.06
24	AB	309	CLA	CHC-C1C	2.17	1.42	1.38
24	BF	503	CLA	C1B-NB	-2.17	1.35	1.37
24	b	613	CLA	CMC-C2C	-2.17	1.46	1.50
24	BE	609	CLA	CMD-C2D	-2.17	1.46	1.50
24	BU	603	CLA	CMC-C2C	-2.17	1.46	1.50
24	Y	315	CLA	CMD-C2D	-2.17	1.46	1.50
24	y	304	CLA	CMD-C2D	-2.17	1.46	1.50
24	N	611	CLA	CMB-C2B	-2.17	1.46	1.50
24	s	613	CLA	CMB-C2B	-2.17	1.46	1.50
24	C	507	CLA	CMC-C2C	-2.17	1.46	1.50
24	BD	410	CLA	CMD-C2D	-2.17	1.46	1.50
24	s	604	CLA	C1B-C2B	2.17	1.48	1.43
24	B	603	CLA	CMB-C2B	-2.17	1.46	1.50
24	r	603	CLA	MG-ND	-2.17	2.01	2.05
24	g	604	CLA	CHC-C1C	2.17	1.42	1.38
24	BJ	604	CLA	CHC-C1C	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	312	CLA	CMD-C2D	-2.17	1.46	1.50
24	v	603	CLA	CMB-C2B	-2.17	1.46	1.50
25	5	615	LUT	C28-C29	-2.17	1.41	1.45
26	BQ	617	NEX	C32-C33	-2.17	1.41	1.45
32	l	101	SQD	O9-S	2.17	1.51	1.45
26	s	616	NEX	C28-C29	-2.17	1.41	1.45
23	A2	609	CHL	MG-NA	-2.17	2.01	2.06
26	7	319	NEX	C32-C33	-2.17	1.41	1.45
24	C	508	CLA	CMC-C2C	-2.17	1.46	1.50
24	AA	312	CLA	CMB-C2B	-2.17	1.46	1.50
24	BE	614	CLA	CMD-C2D	-2.17	1.46	1.50
24	BE	617	CLA	CMD-C2D	-2.17	1.46	1.50
23	5	606	CHL	C3B-C4B	2.17	1.47	1.42
23	7	309	CHL	C1B-NB	-2.17	1.35	1.37
23	A6	606	CHL	MG-NA	-2.17	2.01	2.06
32	l	101	SQD	O7-S	2.17	1.51	1.45
32	BO	101	SQD	O9-S	2.17	1.51	1.45
23	AB	305	CHL	CHB-C4A	-2.17	1.32	1.37
24	AA	304	CLA	CMB-C2B	-2.17	1.46	1.50
24	A2	604	CLA	CMD-C2D	-2.17	1.46	1.50
24	BE	613	CLA	CMC-C2C	-2.17	1.46	1.50
23	y	307	CHL	C4C-C3C	2.17	1.48	1.45
24	BU	610	CLA	CMC-C2C	-2.17	1.46	1.50
23	A2	609	CHL	C1B-C2B	2.17	1.48	1.43
25	9	615	LUT	C12-C13	-2.17	1.41	1.45
28	AA	301	XAT	C38-C25	2.16	1.55	1.51
24	AA	315	CLA	CHC-C1C	2.16	1.42	1.38
24	A6	609	CLA	CHC-C1C	2.16	1.42	1.38
24	8	309	CLA	CHC-C1C	2.16	1.42	1.38
24	S	602	CLA	CMD-C2D	-2.16	1.46	1.50
24	BQ	603	CLA	CHC-C1C	2.16	1.42	1.38
24	9	604	CLA	MG-ND	-2.16	2.01	2.05
24	C	509	CLA	CMD-C2D	-2.16	1.46	1.50
23	9	601	CHL	C1D-ND	-2.16	1.35	1.37
24	1	504	CLA	CMB-C2B	-2.16	1.46	1.50
24	r	609	CLA	C3B-C4B	2.16	1.47	1.42
24	N	612	CLA	CMB-C2B	-2.16	1.46	1.50
23	r	606	CHL	C4C-C3C	2.16	1.48	1.45
23	AA	302	CHL	C1B-C2B	2.16	1.48	1.43
24	BF	508	CLA	MG-ND	-2.16	2.01	2.05
24	S	603	CLA	MG-NB	-2.16	2.01	2.05
24	I	102	CLA	C1B-C2B	2.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	303	CLA	C1B-NB	-2.16	1.35	1.37
24	1	506	CLA	MG-ND	-2.16	2.01	2.05
23	G	608	CHL	C4C-C3C	2.16	1.48	1.45
24	5	604	CLA	MG-ND	-2.16	2.01	2.05
24	9	610	CLA	MG-ND	-2.16	2.01	2.05
24	v	604	CLA	CMD-C2D	-2.16	1.46	1.50
24	BF	510	CLA	CMC-C2C	-2.16	1.46	1.50
23	Au	605	CHL	C1B-NB	-2.16	1.35	1.37
23	r	607	CHL	MG-NA	-2.16	2.01	2.06
24	9	603	CLA	MG-ND	-2.16	2.01	2.05
24	v	610	CLA	CMB-C2B	-2.16	1.46	1.50
23	BU	606	CHL	C4C-C3C	2.16	1.48	1.45
23	9	608	CHL	CHB-C4A	-2.16	1.32	1.37
24	g	604	CLA	MG-NB	-2.16	2.01	2.05
23	Ba	307	CHL	C4C-C3C	2.16	1.48	1.45
24	y	314	CLA	MG-NB	-2.16	2.01	2.05
23	G	601	CHL	C4B-NB	-2.16	1.35	1.37
23	BQ	607	CHL	MG-NA	-2.16	2.01	2.06
24	N	613	CLA	CMC-C2C	-2.16	1.46	1.50
24	n	604	CLA	CMB-C2B	-2.16	1.46	1.50
30	BF	519	LMG	O7-C8	-2.16	1.41	1.46
24	8	302	CLA	MG-ND	-2.16	2.01	2.05
34	A	402	DGD	O1G-C1G	-2.16	1.40	1.45
24	C	510	CLA	CMB-C2B	-2.16	1.46	1.50
24	Au	610	CLA	CMD-C2D	-2.16	1.46	1.50
23	y	302	CHL	C1D-ND	-2.16	1.35	1.37
24	C	504	CLA	CMB-C2B	-2.16	1.46	1.50
29	BF	516	BCR	C38-C26	-2.16	1.47	1.50
24	0	602	CLA	C1B-NB	-2.16	1.35	1.37
24	S	608	CLA	CHC-C1C	2.16	1.42	1.38
24	Y	314	CLA	CMC-C2C	-2.16	1.46	1.50
28	7	318	XAT	C18-C5	2.16	1.55	1.51
24	BJ	614	CLA	MG-NB	-2.16	2.01	2.05
24	G	613	CLA	CMD-C2D	-2.16	1.46	1.50
24	Y	305	CLA	CMC-C2C	-2.16	1.46	1.50
23	BV	601	CHL	C1D-ND	-2.16	1.35	1.37
24	r	611	CLA	MG-ND	-2.16	2.01	2.05
24	9	612	CLA	MG-ND	-2.16	2.01	2.05
23	BB	307	CHL	CHB-C4A	-2.16	1.32	1.37
24	BE	613	CLA	CMB-C2B	-2.16	1.46	1.50
23	5	608	CHL	C4C-C3C	2.16	1.48	1.45
23	G	606	CHL	C4C-C3C	2.16	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	608	CHL	C4C-C3C	2.16	1.48	1.45
24	BJ	603	CLA	MG-NB	-2.15	2.01	2.05
24	B	605	CLA	CMB-C2B	-2.15	1.46	1.50
24	r	610	CLA	C1B-NB	-2.15	1.35	1.37
24	6	603	CLA	MG-ND	-2.15	2.01	2.05
24	S	609	CLA	CMD-C2D	-2.15	1.46	1.50
24	b	617	CLA	CMD-C2D	-2.15	1.46	1.50
24	A2	602	CLA	CMC-C2C	-2.15	1.46	1.50
24	BE	610	CLA	CMC-C2C	-2.15	1.46	1.50
32	R	411	SQD	O7-S	2.15	1.51	1.45
24	G	610	CLA	CMD-C2D	-2.15	1.46	1.50
24	b	611	CLA	CMD-C2D	-2.15	1.46	1.50
24	r	601	CLA	CMB-C2B	-2.15	1.46	1.50
24	v	602	CLA	CMD-C2D	-2.15	1.46	1.50
24	BF	514	CLA	CMD-C2D	-2.15	1.46	1.50
23	7	309	CHL	C1D-ND	-2.15	1.35	1.37
24	A	407	CLA	CMB-C2B	-2.15	1.46	1.50
24	BV	613	CLA	CMD-C2D	-2.15	1.46	1.50
24	R	406	CLA	CMB-C2B	-2.15	1.46	1.50
24	c	508	CLA	MG-ND	-2.15	2.01	2.05
24	r	608	CLA	MG-ND	-2.15	2.01	2.05
24	b	606	CLA	CHC-C1C	2.15	1.42	1.38
23	n	609	CHL	C4C-C3C	2.15	1.48	1.45
24	BU	609	CLA	C3B-C4B	2.15	1.47	1.42
23	6	607	CHL	CHB-C4A	-2.15	1.32	1.37
23	0	607	CHL	CHB-C4A	-2.15	1.32	1.37
24	A6	612	CLA	CMD-C2D	-2.15	1.46	1.50
24	1	505	CLA	CMC-C2C	-2.15	1.46	1.50
24	BJ	611	CLA	MG-NB	-2.15	2.01	2.05
24	BU	612	CLA	C1B-NB	-2.15	1.35	1.37
24	B	604	CLA	CMD-C2D	-2.15	1.46	1.50
24	R	405	CLA	CMB-C2B	-2.15	1.46	1.50
23	Y	302	CHL	C4B-NB	-2.15	1.35	1.37
23	Au	609	CHL	C1D-ND	-2.15	1.35	1.37
24	c	503	CLA	CMD-C2D	-2.15	1.46	1.50
24	S	604	CLA	CMB-C2B	-2.15	1.46	1.50
23	AB	307	CHL	C4C-C3C	2.15	1.48	1.45
24	5	611	CLA	CHC-C1C	2.15	1.42	1.38
24	b	610	CLA	CMC-C2C	-2.15	1.46	1.50
24	BF	513	CLA	CMC-C2C	-2.15	1.46	1.50
29	4	101	BCR	C33-C5	-2.15	1.47	1.50
24	6	602	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	601	CLA	CMD-C2D	-2.15	1.46	1.50
24	9	603	CLA	CMB-C2B	-2.15	1.46	1.50
24	9	611	CLA	CMD-C2D	-2.15	1.46	1.50
23	BU	607	CHL	MG-NA	-2.15	2.01	2.06
24	6	610	CLA	CHC-C1C	2.15	1.42	1.38
32	D	406	SQD	O9-S	2.15	1.51	1.45
24	Ba	312	CLA	CMD-C2D	-2.15	1.46	1.50
24	Ba	313	CLA	CMC-C2C	-2.15	1.46	1.50
24	b	603	CLA	CHC-C1C	2.15	1.42	1.38
24	g	611	CLA	CHC-C1C	2.15	1.42	1.38
26	s	616	NEX	C32-C33	-2.15	1.41	1.45
23	8	304	CHL	C1D-ND	-2.15	1.35	1.37
24	0	613	CLA	C1B-NB	-2.15	1.35	1.37
24	BB	311	CLA	C1B-NB	-2.15	1.35	1.37
24	BE	604	CLA	CMB-C2B	-2.15	1.46	1.50
23	BV	601	CHL	C4C-C3C	2.15	1.48	1.45
24	BE	609	CLA	C3B-C4B	2.15	1.47	1.42
23	r	607	CHL	CHB-C4A	-2.15	1.32	1.37
24	A6	608	CLA	CHC-C1C	2.15	1.42	1.38
24	7	312	CLA	CMB-C2B	-2.15	1.46	1.50
24	v	615	CLA	CMD-C2D	-2.15	1.46	1.50
24	BE	608	CLA	CMD-C2D	-2.15	1.46	1.50
23	BJ	606	CHL	C1B-NB	-2.15	1.35	1.37
23	r	606	CHL	CHB-C4A	-2.15	1.32	1.37
23	BU	606	CHL	CHB-C4A	-2.15	1.32	1.37
24	b	609	CLA	CMD-C2D	-2.15	1.46	1.50
24	C	506	CLA	CMC-C2C	-2.15	1.46	1.50
24	v	604	CLA	CMC-C2C	-2.15	1.46	1.50
24	BU	614	CLA	CMD-C2D	-2.15	1.46	1.50
23	S	606	CHL	C4B-NB	-2.15	1.35	1.37
24	5	604	CLA	C1B-NB	-2.15	1.35	1.37
24	0	603	CLA	C1B-NB	-2.15	1.35	1.37
32	BG	406	SQD	O7-S	2.15	1.51	1.45
25	5	615	LUT	C12-C13	-2.15	1.41	1.45
23	6	607	CHL	C4C-C3C	2.15	1.48	1.45
23	Au	609	CHL	MG-NA	-2.15	2.01	2.06
23	9	606	CHL	C1D-ND	-2.14	1.35	1.37
24	BB	303	CLA	C4B-NB	2.14	1.40	1.37
24	Au	612	CLA	CMD-C2D	-2.14	1.46	1.50
24	BG	401	CLA	CMC-C2C	-2.14	1.46	1.50
32	L	103	SQD	O7-S	2.14	1.51	1.45
32	L	103	SQD	O9-S	2.14	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	614	CLA	CMC-C2C	-2.14	1.46	1.50
24	5	603	CLA	MG-ND	-2.14	2.01	2.05
32	A	413	SQD	O7-S	2.14	1.51	1.45
24	B	607	CLA	CMD-C2D	-2.14	1.46	1.50
24	r	612	CLA	CMD-C2D	-2.14	1.46	1.50
24	A2	612	CLA	CMC-C2C	-2.14	1.46	1.50
24	A6	609	CLA	CMC-C2C	-2.14	1.46	1.50
24	BU	611	CLA	CMC-C2C	-2.14	1.46	1.50
23	9	601	CHL	CHB-C4A	-2.14	1.32	1.37
24	v	616	CLA	CMD-C2D	-2.14	1.46	1.50
24	Au	610	CLA	CMB-C2B	-2.14	1.46	1.50
24	1	506	CLA	CMC-C2C	-2.14	1.46	1.50
24	Y	313	CLA	CMC-C2C	-2.14	1.46	1.50
24	s	602	CLA	CMD-C2D	-2.14	1.46	1.50
24	b	615	CLA	CMD-C2D	-2.14	1.46	1.50
24	y	313	CLA	CMB-C2B	-2.14	1.46	1.50
24	BJ	610	CLA	MG-NB	-2.14	2.01	2.05
24	B	606	CLA	CMB-C2B	-2.14	1.46	1.50
24	D	401	CLA	CMB-C2B	-2.14	1.46	1.50
24	r	614	CLA	CMD-C2D	-2.14	1.46	1.50
24	Au	613	CLA	CMD-C2D	-2.14	1.46	1.50
24	0	614	CLA	CMB-C2B	-2.14	1.46	1.50
24	BU	614	CLA	CMC-C2C	-2.14	1.46	1.50
24	b	607	CLA	MG-NB	-2.14	2.01	2.05
24	C	513	CLA	CMB-C2B	-2.14	1.46	1.50
24	BV	602	CLA	CMD-C2D	-2.14	1.46	1.50
23	8	306	CHL	C1B-C2B	2.14	1.48	1.43
24	B	603	CLA	CHC-C1C	2.14	1.42	1.38
30	BE	621	LMG	O7-C8	-2.14	1.41	1.46
24	AB	308	CLA	MG-ND	-2.14	2.01	2.05
23	n	606	CHL	MG-NA	-2.14	2.01	2.06
23	A6	605	CHL	C1B-NB	-2.14	1.35	1.37
23	Ba	307	CHL	C4B-NB	-2.14	1.35	1.37
24	B	603	CLA	CMD-C2D	-2.14	1.46	1.50
24	BF	507	CLA	CMC-C2C	-2.14	1.46	1.50
23	Y	302	CHL	CHB-C4A	-2.14	1.32	1.37
24	5	611	CLA	CMD-C2D	-2.14	1.46	1.50
24	9	602	CLA	CMB-C2B	-2.14	1.46	1.50
24	BE	612	CLA	CMC-C2C	-2.14	1.46	1.50
32	L	101	SQD	O7-S	2.14	1.51	1.45
23	G	609	CHL	C1B-NB	-2.14	1.35	1.37
23	Ba	309	CHL	C1D-ND	-2.14	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	605	CHL	C4C-C3C	2.14	1.48	1.45
24	6	614	CLA	CMD-C2D	-2.14	1.46	1.50
26	G	617	NEX	C28-C29	-2.14	1.41	1.45
24	BJ	604	CLA	MG-NB	-2.14	2.01	2.05
24	Aw	102	CLA	CMC-C2C	-2.14	1.46	1.50
28	9	619	XAT	C20-C13	2.14	1.55	1.50
33	f	102	HEM	FE-NC	2.14	2.02	1.95
24	G	602	CLA	CMD-C2D	-2.14	1.46	1.50
24	BE	605	CLA	CMD-C2D	-2.14	1.46	1.50
23	A2	601	CHL	C1D-ND	-2.14	1.35	1.37
24	S	613	CLA	CMB-C2B	-2.14	1.46	1.50
24	v	614	CLA	CMB-C2B	-2.14	1.46	1.50
24	BJ	613	CLA	CHC-C1C	2.14	1.42	1.38
23	9	601	CHL	C4B-NB	-2.14	1.35	1.37
24	G	612	CLA	CMD-C2D	-2.14	1.46	1.50
24	BU	604	CLA	MG-ND	-2.14	2.01	2.05
24	r	604	CLA	MG-ND	-2.14	2.01	2.05
24	5	603	CLA	CMB-C2B	-2.13	1.46	1.50
24	b	604	CLA	CMB-C2B	-2.13	1.46	1.50
24	A6	610	CLA	CMD-C2D	-2.13	1.46	1.50
24	BQ	613	CLA	CMD-C2D	-2.13	1.46	1.50
24	6	604	CLA	C3C-C2C	2.13	1.41	1.36
24	r	611	CLA	CMC-C2C	-2.13	1.46	1.50
24	v	605	CLA	CMC-C2C	-2.13	1.46	1.50
23	5	605	CHL	C4C-C3C	2.13	1.48	1.45
24	BB	314	CLA	MG-ND	-2.13	2.01	2.05
23	G	605	CHL	C1B-NB	-2.13	1.35	1.37
23	y	310	CHL	C1B-NB	-2.13	1.35	1.37
24	BE	607	CLA	MG-NB	-2.13	2.01	2.05
24	8	308	CLA	CHC-C1C	2.13	1.42	1.38
24	2	402	CLA	CMB-C2B	-2.13	1.46	1.50
24	BG	402	CLA	CMD-C2D	-2.13	1.46	1.50
23	n	607	CHL	MG-NA	-2.13	2.01	2.06
24	BU	601	CLA	C1B-C2B	2.13	1.48	1.43
24	Aw	102	CLA	MG-ND	-2.13	2.01	2.05
24	Ba	304	CLA	CHC-C1C	2.13	1.42	1.38
23	Au	606	CHL	C4C-C3C	2.13	1.48	1.45
24	5	610	CLA	C1B-NB	-2.13	1.35	1.37
24	s	602	CLA	MG-NB	-2.13	2.01	2.05
24	S	610	CLA	CMD-C2D	-2.13	1.46	1.50
24	y	313	CLA	CMC-C2C	-2.13	1.46	1.50
24	A6	609	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	0	606	CHL	MG-NA	-2.13	2.01	2.06
24	g	603	CLA	MG-NB	-2.13	2.01	2.05
24	G	611	CLA	CMB-C2B	-2.13	1.46	1.50
24	C	513	CLA	CMD-C2D	-2.13	1.46	1.50
24	BJ	602	CLA	CHC-C1C	2.13	1.42	1.38
24	BB	303	CLA	MG-ND	-2.13	2.01	2.05
24	d	402	CLA	CMD-C2D	-2.13	1.46	1.50
24	r	603	CLA	CMC-C2C	-2.13	1.46	1.50
23	5	608	CHL	CHB-C4A	-2.13	1.32	1.37
23	g	606	CHL	C1B-NB	-2.13	1.35	1.37
23	AB	306	CHL	C1B-C2B	2.13	1.48	1.43
24	A2	613	CLA	CMC-C2C	-2.13	1.46	1.50
24	A6	604	CLA	CMC-C2C	-2.13	1.46	1.50
24	BE	609	CLA	CMB-C2B	-2.13	1.46	1.50
24	Ba	304	CLA	CMD-C2D	-2.13	1.46	1.50
32	d	406	SQD	O7-S	2.13	1.51	1.45
26	g	617	NEX	C28-C29	-2.13	1.41	1.45
23	9	606	CHL	C3B-C4B	2.13	1.47	1.42
24	C	505	CLA	CMC-C2C	-2.13	1.46	1.50
24	A6	610	CLA	CMB-C2B	-2.13	1.46	1.50
23	9	607	CHL	C1B-C2B	2.13	1.48	1.43
24	AB	303	CLA	MG-ND	-2.13	2.01	2.05
24	BJ	613	CLA	MG-NB	-2.13	2.01	2.05
24	N	612	CLA	CMC-C2C	-2.13	1.46	1.50
24	0	603	CLA	CMD-C2D	-2.13	1.46	1.50
24	BE	615	CLA	CMB-C2B	-2.13	1.46	1.50
23	Au	606	CHL	MG-NA	-2.13	2.01	2.06
23	5	601	CHL	C4B-NB	-2.13	1.35	1.37
30	2	407	LMG	O7-C8	-2.13	1.41	1.46
23	G	607	CHL	C4C-C3C	2.13	1.48	1.45
23	9	605	CHL	C4C-C3C	2.13	1.48	1.45
34	1	518	DGD	O1G-C1G	-2.13	1.40	1.45
24	D	402	CLA	CMD-C2D	-2.13	1.46	1.50
26	BV	616	NEX	C12-C13	-2.13	1.41	1.45
24	AB	302	CLA	MG-ND	-2.13	2.01	2.05
24	g	612	CLA	CHC-C1C	2.13	1.42	1.38
27	BJ	618	LHG	O7-C5	-2.13	1.41	1.46
28	7	301	XAT	C38-C25	2.13	1.55	1.51
24	G	603	CLA	CMB-C2B	-2.13	1.46	1.50
24	0	614	CLA	CMD-C2D	-2.13	1.46	1.50
24	AB	308	CLA	C1B-C2B	2.13	1.48	1.43
24	6	611	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CMC-C2C	-2.13	1.46	1.50
24	v	603	CLA	CMD-C2D	-2.13	1.46	1.50
24	5	610	CLA	MG-ND	-2.13	2.01	2.05
24	r	610	CLA	MG-ND	-2.13	2.01	2.05
24	g	603	CLA	CMD-C2D	-2.13	1.46	1.50
24	A2	604	CLA	CMC-C2C	-2.13	1.46	1.50
24	A6	603	CLA	CMD-C2D	-2.13	1.46	1.50
24	g	602	CLA	CHC-C1C	2.13	1.42	1.38
24	b	607	CLA	CMB-C2B	-2.13	1.46	1.50
24	BE	607	CLA	CMB-C2B	-2.13	1.46	1.50
23	G	606	CHL	MG-NA	-2.13	2.01	2.06
24	Au	613	CLA	CMB-C2B	-2.13	1.46	1.50
24	BU	614	CLA	CMB-C2B	-2.13	1.46	1.50
23	6	601	CHL	C1B-C2B	2.12	1.48	1.43
23	BB	310	CHL	C1B-C2B	2.12	1.48	1.43
24	D	401	CLA	MG-ND	-2.12	2.01	2.05
24	b	614	CLA	CMD-C2D	-2.12	1.46	1.50
24	a	407	CLA	CMB-C2B	-2.12	1.46	1.50
24	AB	301	CLA	CMB-C2B	-2.12	1.46	1.50
24	BJ	603	CLA	CMD-C2D	-2.12	1.46	1.50
24	6	614	CLA	MG-ND	-2.12	2.01	2.05
24	B	609	CLA	CMD-C2D	-2.12	1.46	1.50
24	Au	611	CLA	CMB-C2B	-2.12	1.46	1.50
24	N	612	CLA	CHC-C1C	2.12	1.42	1.38
24	BU	610	CLA	MG-ND	-2.12	2.01	2.05
24	BF	508	CLA	C3B-C4B	2.12	1.47	1.42
24	B	614	CLA	CMB-C2B	-2.12	1.46	1.50
24	1	502	CLA	CMC-C2C	-2.12	1.46	1.50
24	1	511	CLA	CHC-C1C	2.12	1.42	1.38
24	n	603	CLA	MG-NB	-2.12	2.01	2.05
24	BF	512	CLA	C1B-NB	-2.12	1.35	1.37
24	S	612	CLA	CMD-C2D	-2.12	1.46	1.50
31	2	404	PL9	C20-C19	-2.12	1.45	1.50
24	b	614	CLA	CMC-C2C	-2.12	1.46	1.50
24	BB	315	CLA	CMC-C2C	-2.12	1.46	1.50
23	Au	607	CHL	C1D-ND	-2.12	1.35	1.37
24	C	510	CLA	CMC-C2C	-2.12	1.46	1.50
24	BB	304	CLA	CMC-C2C	-2.12	1.46	1.50
24	BF	509	CLA	CMD-C2D	-2.12	1.46	1.50
24	B	601	CLA	MG-NB	-2.12	2.01	2.05
29	8	313	BCR	C33-C5	-2.12	1.47	1.50
24	y	304	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Ba	303	CLA	MG-NB	-2.12	2.01	2.05
24	B	602	CLA	CMD-C2D	-2.12	1.46	1.50
24	Y	303	CLA	CMC-C2C	-2.12	1.46	1.50
24	BB	312	CLA	CMC-C2C	-2.12	1.46	1.50
24	n	614	CLA	CHC-C1C	2.12	1.42	1.38
23	A6	605	CHL	C4C-C3C	2.12	1.48	1.45
24	0	611	CLA	MG-ND	-2.12	2.01	2.05
24	b	603	CLA	CMD-C2D	-2.12	1.46	1.50
24	2	403	CLA	CMD-C2D	-2.12	1.46	1.50
24	A6	608	CLA	CMD-C2D	-2.12	1.46	1.50
23	5	601	CHL	CHB-C4A	-2.12	1.32	1.37
34	C	518	DGD	O1G-C1G	-2.12	1.40	1.45
34	a	413	DGD	O2G-C2G	-2.12	1.41	1.46
23	y	307	CHL	C4B-NB	-2.12	1.35	1.37
24	BV	608	CLA	CHC-C1C	2.12	1.42	1.38
29	R	410	BCR	C33-C5	-2.12	1.47	1.50
24	B	605	CLA	CMC-C2C	-2.12	1.46	1.50
24	b	612	CLA	CMB-C2B	-2.12	1.46	1.50
24	BB	314	CLA	CMD-C2D	-2.12	1.46	1.50
23	AA	309	CHL	C1D-ND	-2.12	1.35	1.37
24	v	601	CLA	MG-NB	-2.12	2.01	2.05
24	b	602	CLA	CMD-C2D	-2.12	1.46	1.50
24	Au	614	CLA	CMB-C2B	-2.12	1.46	1.50
23	BQ	609	CHL	C4C-C3C	2.12	1.48	1.45
24	v	606	CLA	CMB-C2B	-2.12	1.46	1.50
24	BF	511	CLA	C1B-NB	-2.12	1.35	1.37
24	G	613	CLA	CMC-C2C	-2.12	1.46	1.50
24	d	401	CLA	CMB-C2B	-2.12	1.46	1.50
24	BU	612	CLA	CMC-C2C	-2.12	1.46	1.50
24	g	613	CLA	CHC-C1C	2.12	1.42	1.38
23	0	605	CHL	C4C-C3C	2.12	1.48	1.45
24	v	607	CLA	CMC-C2C	-2.12	1.46	1.50
24	v	615	CLA	CMB-C2B	-2.12	1.46	1.50
24	BD	405	CLA	CMC-C2C	-2.12	1.46	1.50
24	n	603	CLA	CHC-C1C	2.12	1.42	1.38
32	2	408	SQD	C44-C45	2.12	1.57	1.50
23	y	308	CHL	C4B-NB	-2.11	1.35	1.37
23	Au	608	CHL	C4C-C3C	2.11	1.48	1.45
23	s	605	CHL	MG-NA	-2.11	2.01	2.06
24	5	602	CLA	CMB-C2B	-2.11	1.46	1.50
24	6	614	CLA	CMB-C2B	-2.11	1.46	1.50
24	N	604	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	CMC-C2C	-2.11	1.46	1.50
32	A1	101	SQD	O9-S	2.11	1.51	1.45
24	n	613	CLA	CMD-C2D	-2.11	1.46	1.50
23	6	609	CHL	C4C-C3C	2.11	1.48	1.45
26	BJ	617	NEX	C28-C29	-2.11	1.41	1.45
23	S	606	CHL	C1D-ND	-2.11	1.35	1.37
24	Y	314	CLA	MG-ND	-2.11	2.01	2.05
23	0	601	CHL	C1B-C2B	2.11	1.48	1.43
24	AA	315	CLA	CMB-C2B	-2.11	1.46	1.50
24	B	610	CLA	CMB-C2B	-2.11	1.46	1.50
23	g	608	CHL	C1B-NB	-2.11	1.35	1.37
23	BJ	608	CHL	C1B-NB	-2.11	1.35	1.37
23	Ba	310	CHL	C4B-NB	-2.11	1.35	1.37
32	2	408	SQD	O9-S	2.11	1.51	1.45
23	6	606	CHL	MG-NA	-2.11	2.01	2.06
24	s	613	CLA	CMD-C2D	-2.11	1.46	1.50
24	Ba	315	CLA	CMD-C2D	-2.11	1.46	1.50
32	A1	101	SQD	O7-S	2.11	1.51	1.45
24	n	612	CLA	CHC-C1C	2.11	1.42	1.38
23	n	608	CHL	C1D-ND	-2.11	1.35	1.37
24	C	505	CLA	CMB-C2B	-2.11	1.46	1.50
26	BJ	617	NEX	C32-C33	-2.11	1.41	1.45
24	c	504	CLA	MG-ND	-2.11	2.01	2.05
24	AB	301	CLA	CBD-CAD	2.11	1.56	1.51
24	6	604	CLA	CMB-C2B	-2.11	1.46	1.50
26	BV	616	NEX	C32-C33	-2.11	1.41	1.45
32	Az	101	SQD	O7-S	2.11	1.51	1.45
24	BU	608	CLA	MG-ND	-2.11	2.01	2.05
24	N	602	CLA	CMC-C2C	-2.11	1.46	1.50
24	BQ	614	CLA	CHC-C1C	2.11	1.42	1.38
23	G	607	CHL	MG-NA	-2.11	2.01	2.06
24	g	610	CLA	MG-NB	-2.11	2.01	2.05
24	c	503	CLA	MG-ND	-2.11	2.01	2.05
24	I	102	CLA	CMC-C2C	-2.11	1.46	1.50
24	S	609	CLA	CMB-C2B	-2.11	1.46	1.50
24	b	608	CLA	CMD-C2D	-2.11	1.46	1.50
24	A6	612	CLA	CMC-C2C	-2.11	1.46	1.50
24	a	405	CLA	CHC-C1C	2.11	1.42	1.38
24	1	513	CLA	CMD-C2D	-2.11	1.46	1.50
24	BB	305	CLA	MG-ND	-2.11	2.01	2.05
24	BE	613	CLA	MG-ND	-2.11	2.01	2.05
24	c	503	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	611	CLA	CHC-C1C	2.11	1.42	1.38
24	Y	314	CLA	CMD-C2D	-2.11	1.46	1.50
24	a	405	CLA	CMC-C2C	-2.11	1.46	1.50
24	0	604	CLA	CMB-C2B	-2.11	1.46	1.50
24	v	608	CLA	CMC-C2C	-2.11	1.46	1.50
24	Au	602	CLA	CHC-C1C	2.11	1.42	1.38
32	BD	412	SQD	O7-S	2.11	1.51	1.45
23	Au	606	CHL	C1D-ND	-2.11	1.35	1.37
24	6	613	CLA	C1B-NB	-2.11	1.35	1.37
24	G	613	CLA	CMB-C2B	-2.11	1.46	1.50
24	0	602	CLA	C1B-C2B	2.11	1.48	1.43
24	BE	606	CLA	CMB-C2B	-2.11	1.46	1.50
24	y	303	CLA	MG-NB	-2.11	2.01	2.05
23	G	607	CHL	CHB-C4A	-2.11	1.32	1.37
24	r	601	CLA	CMC-C2C	-2.11	1.46	1.50
23	Y	308	CHL	MG-NA	-2.11	2.01	2.06
24	Au	613	CLA	CMC-C2C	-2.11	1.46	1.50
24	g	614	CLA	CHC-C1C	2.10	1.42	1.38
24	S	610	CLA	CMB-C2B	-2.10	1.46	1.50
24	r	604	CLA	CMB-C2B	-2.10	1.46	1.50
24	AB	301	CLA	C1B-NB	-2.10	1.35	1.37
24	BF	507	CLA	C1B-C2B	2.10	1.48	1.43
24	AA	313	CLA	CHC-C1C	2.10	1.42	1.38
24	BQ	603	CLA	MG-NB	-2.10	2.01	2.05
34	a	413	DGD	O1G-C1G	-2.10	1.40	1.45
29	A	411	BCR	C33-C5	-2.10	1.47	1.50
24	6	603	CLA	CMD-C2D	-2.10	1.46	1.50
24	S	603	CLA	CMD-C2D	-2.10	1.46	1.50
23	Y	307	CHL	C1B-C2B	2.10	1.48	1.43
24	AA	305	CLA	CHC-C1C	2.10	1.42	1.38
24	BQ	612	CLA	MG-NB	-2.10	2.01	2.05
38	BD	409	PHO	C3B-CAB	-2.10	1.43	1.47
24	b	612	CLA	CMC-C2C	-2.10	1.46	1.50
24	BV	611	CLA	CMB-C2B	-2.10	1.46	1.50
24	Y	315	CLA	CMC-C2C	-2.10	1.46	1.50
24	n	602	CLA	CMD-C2D	-2.10	1.46	1.50
24	7	305	CLA	CHC-C1C	2.10	1.42	1.38
24	Y	303	CLA	MG-ND	-2.10	2.01	2.05
24	n	610	CLA	MG-NB	-2.10	2.01	2.05
24	C	512	CLA	CMC-C2C	-2.10	1.46	1.50
24	c	502	CLA	CMC-C2C	-2.10	1.46	1.50
32	D	406	SQD	O7-S	2.10	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	305	CHL	C4C-C3C	2.10	1.48	1.45
24	A6	613	CLA	CMB-C2B	-2.10	1.46	1.50
24	A2	614	CLA	CMD-C2D	-2.10	1.46	1.50
24	BU	611	CLA	C1B-NB	-2.10	1.35	1.37
24	y	311	CLA	CMB-C2B	-2.10	1.46	1.50
24	BE	603	CLA	CMB-C2B	-2.10	1.46	1.50
24	BF	513	CLA	C1B-NB	-2.10	1.35	1.37
24	1	507	CLA	MG-ND	-2.10	2.01	2.05
23	Au	607	CHL	MG-NA	-2.10	2.01	2.06
24	Ba	311	CLA	CMB-C2B	-2.10	1.46	1.50
24	g	614	CLA	MG-NB	-2.10	2.01	2.05
24	BV	602	CLA	MG-NB	-2.10	2.01	2.05
23	r	605	CHL	C1D-ND	-2.10	1.35	1.37
24	S	603	CLA	CHC-C1C	2.10	1.42	1.38
24	BD	405	CLA	CMB-C2B	-2.10	1.46	1.50
24	g	613	CLA	MG-NB	-2.10	2.01	2.05
23	N	607	CHL	C4C-C3C	2.10	1.48	1.45
24	B	607	CLA	CMC-C2C	-2.10	1.46	1.50
24	N	614	CLA	MG-NB	-2.10	2.01	2.05
23	g	607	CHL	C4B-NB	-2.10	1.35	1.37
24	BQ	611	CLA	CHC-C1C	2.10	1.42	1.38
32	a	412	SQD	O7-S	2.10	1.51	1.45
24	BQ	610	CLA	MG-NB	-2.10	2.01	2.05
24	d	402	CLA	CMB-C2B	-2.10	1.46	1.50
27	g	618	LHG	O7-C5	-2.10	1.41	1.46
24	5	612	CLA	MG-ND	-2.10	2.01	2.05
24	A2	614	CLA	MG-NB	-2.10	2.01	2.05
28	y	301	XAT	C38-C25	2.10	1.55	1.51
24	Y	303	CLA	C1B-NB	-2.10	1.35	1.37
24	r	612	CLA	CMC-C2C	-2.10	1.46	1.50
24	A6	610	CLA	CMC-C2C	-2.10	1.46	1.50
24	B	616	CLA	CMD-C2D	-2.09	1.46	1.50
23	BB	310	CHL	CHB-C4A	-2.09	1.32	1.37
24	C	508	CLA	C1B-NB	-2.09	1.35	1.37
24	n	612	CLA	MG-NB	-2.09	2.01	2.05
24	b	606	CLA	CMB-C2B	-2.09	1.46	1.50
23	g	607	CHL	C1B-NB	-2.09	1.35	1.37
23	Au	601	CHL	CHB-C4A	-2.09	1.32	1.37
24	N	610	CLA	CMD-C2D	-2.09	1.46	1.50
24	BQ	602	CLA	CMD-C2D	-2.09	1.46	1.50
24	8	303	CLA	MG-ND	-2.09	2.01	2.05
24	Ba	305	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	606	CHL	C1B-NB	-2.09	1.35	1.37
23	s	607	CHL	C1B-NB	-2.09	1.35	1.37
23	BB	307	CHL	C4B-NB	-2.09	1.35	1.37
24	b	616	CLA	CHC-C1C	2.09	1.42	1.38
24	7	303	CLA	CMB-C2B	-2.09	1.46	1.50
24	G	614	CLA	CMB-C2B	-2.09	1.46	1.50
24	c	509	CLA	CMD-C2D	-2.09	1.46	1.50
24	BE	602	CLA	CMD-C2D	-2.09	1.46	1.50
24	b	604	CLA	CHC-C1C	2.09	1.42	1.38
24	n	613	CLA	CHC-C1C	2.09	1.42	1.38
23	g	607	CHL	CHB-C4A	-2.09	1.32	1.37
24	s	608	CLA	CHC-C1C	2.09	1.42	1.38
23	5	607	CHL	C1B-C2B	2.09	1.48	1.43
24	y	315	CLA	CMD-C2D	-2.09	1.46	1.50
24	BB	305	CLA	CMD-C2D	-2.09	1.46	1.50
23	BQ	606	CHL	C4B-NB	-2.09	1.35	1.37
24	c	512	CLA	C1B-NB	-2.09	1.35	1.37
24	9	613	CLA	MG-ND	-2.09	2.01	2.05
23	G	601	CHL	C4C-C3C	2.09	1.48	1.45
24	b	604	CLA	CMD-C2D	-2.09	1.46	1.50
24	2	402	CLA	MG-ND	-2.09	2.01	2.05
24	N	611	CLA	CMC-C2C	-2.09	1.46	1.50
24	0	602	CLA	CMC-C2C	-2.09	1.46	1.50
23	G	609	CHL	C1D-ND	-2.09	1.35	1.37
23	G	606	CHL	CHB-C4A	-2.09	1.32	1.37
24	8	301	CLA	CMD-C2D	-2.09	1.46	1.50
24	a	406	CLA	CMC-C2C	-2.09	1.46	1.50
23	AB	304	CHL	C4C-C3C	2.09	1.48	1.45
24	v	606	CLA	CHC-C1C	2.09	1.42	1.38
24	AB	301	CLA	CMD-C2D	-2.09	1.46	1.50
24	v	602	CLA	CMC-C2C	-2.09	1.46	1.50
24	BE	614	CLA	CMC-C2C	-2.09	1.46	1.50
23	AA	308	CHL	C4C-C3C	2.09	1.48	1.45
24	n	611	CLA	CHC-C1C	2.09	1.42	1.38
24	A2	611	CLA	CMC-C2C	-2.09	1.46	1.50
24	BF	505	CLA	CMD-C2D	-2.09	1.46	1.50
23	Y	308	CHL	CHB-C4A	-2.09	1.32	1.37
24	BQ	611	CLA	MG-NB	-2.09	2.01	2.05
24	b	605	CLA	CMD-C2D	-2.09	1.46	1.50
24	b	615	CLA	CMB-C2B	-2.09	1.46	1.50
24	n	603	CLA	CMD-C2D	-2.09	1.46	1.50
24	y	311	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	508	CLA	MG-ND	-2.09	2.01	2.05
24	g	612	CLA	CMB-C2B	-2.09	1.46	1.50
24	A6	603	CLA	CHC-C1C	2.09	1.42	1.38
24	r	611	CLA	C1B-NB	-2.09	1.35	1.37
24	7	315	CLA	CMB-C2B	-2.09	1.46	1.50
23	N	601	CHL	C4C-C3C	2.08	1.48	1.45
25	BJ	616	LUT	C8-C9	-2.08	1.41	1.45
24	BF	504	CLA	MG-ND	-2.08	2.01	2.05
24	v	601	CLA	CHC-C1C	2.08	1.42	1.38
23	BJ	607	CHL	CHB-C4A	-2.08	1.32	1.37
23	BQ	608	CHL	C1D-ND	-2.08	1.35	1.37
28	r	616	XAT	C38-C25	2.08	1.55	1.51
24	B	615	CLA	CMB-C2B	-2.08	1.46	1.50
24	R	405	CLA	CMC-C2C	-2.08	1.46	1.50
24	7	314	CLA	MG-ND	-2.08	2.01	2.05
24	v	601	CLA	CMD-C2D	-2.08	1.46	1.50
24	v	613	CLA	CMC-C2C	-2.08	1.46	1.50
23	BU	605	CHL	C1D-ND	-2.08	1.35	1.37
24	v	604	CLA	C1B-NB	-2.08	1.35	1.37
24	b	612	CLA	CHC-C1C	2.08	1.42	1.38
24	5	613	CLA	MG-ND	-2.08	2.01	2.05
34	BD	413	DGD	O2G-C2G	-2.08	1.41	1.46
24	v	608	CLA	CMD-C2D	-2.08	1.46	1.50
24	BV	609	CLA	CMD-C2D	-2.08	1.46	1.50
23	A2	609	CHL	CHB-C4A	-2.08	1.32	1.37
24	A	407	CLA	CHC-C1C	2.08	1.42	1.38
24	A2	612	CLA	CHC-C1C	2.08	1.42	1.38
24	A2	604	CLA	C1B-NB	-2.08	1.35	1.37
23	Y	310	CHL	C4C-C3C	2.08	1.48	1.45
26	BQ	617	NEX	C12-C13	-2.08	1.41	1.45
24	b	603	CLA	CMB-C2B	-2.08	1.46	1.50
24	Au	612	CLA	CMB-C2B	-2.08	1.46	1.50
24	g	603	CLA	CHC-C1C	2.08	1.42	1.38
24	BJ	603	CLA	CHC-C1C	2.08	1.42	1.38
27	w	201	LHG	O7-C5	-2.08	1.41	1.46
23	S	607	CHL	C4B-NB	-2.08	1.35	1.37
24	6	603	CLA	C1B-NB	-2.08	1.35	1.37
24	0	610	CLA	C1B-C2B	2.08	1.48	1.43
23	G	601	CHL	CHB-C4A	-2.08	1.32	1.37
24	1	511	CLA	CMC-C2C	-2.08	1.46	1.50
24	I	102	CLA	MG-ND	-2.08	2.01	2.05
24	8	301	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	301	CLA	CBD-CAD	2.08	1.56	1.51
38	R	408	PHO	C3B-CAB	-2.08	1.43	1.47
24	Ba	311	CLA	CMC-C2C	-2.08	1.46	1.50
32	l	102	SQD	O7-S	2.08	1.51	1.45
24	c	507	CLA	CHC-C1C	2.08	1.42	1.38
24	BJ	612	CLA	CHC-C1C	2.08	1.42	1.38
24	Au	603	CLA	CMC-C2C	-2.08	1.46	1.50
24	BE	615	CLA	CMC-C2C	-2.08	1.46	1.50
23	0	609	CHL	C2C-C1C	2.08	1.49	1.44
24	v	609	CLA	MG-ND	-2.08	2.01	2.05
24	S	609	CLA	CMC-C2C	-2.08	1.46	1.50
24	v	601	CLA	CMB-C2B	-2.08	1.46	1.50
23	BQ	607	CHL	C4B-NB	-2.08	1.35	1.37
24	BF	505	CLA	CMC-C2C	-2.08	1.46	1.50
24	s	611	CLA	CMB-C2B	-2.08	1.46	1.50
26	y	318	NEX	C12-C13	-2.08	1.41	1.45
32	BO	102	SQD	O7-S	2.08	1.51	1.45
24	BF	513	CLA	MG-ND	-2.08	2.01	2.05
24	7	315	CLA	CMD-C2D	-2.08	1.46	1.50
24	AA	303	CLA	CMB-C2B	-2.08	1.46	1.50
23	BJ	605	CHL	MG-NA	-2.08	2.01	2.06
29	Bb	101	BCR	C38-C26	-2.08	1.47	1.50
24	v	607	CLA	CMB-C2B	-2.08	1.46	1.50
23	AB	305	CHL	C4C-C3C	2.08	1.48	1.45
24	C	511	CLA	CHC-C1C	2.08	1.42	1.38
24	BG	402	CLA	CMB-C2B	-2.08	1.46	1.50
23	G	607	CHL	C1D-ND	-2.08	1.35	1.37
24	6	602	CLA	C4B-NB	2.08	1.40	1.37
24	Y	313	CLA	MG-ND	-2.08	2.01	2.05
24	C	502	CLA	CMC-C2C	-2.08	1.46	1.50
24	BD	406	CLA	CMC-C2C	-2.08	1.46	1.50
24	v	613	CLA	CHC-C1C	2.07	1.42	1.38
24	v	602	CLA	CMB-C2B	-2.07	1.46	1.50
33	BI	102	HEM	CMB-C2B	2.07	1.55	1.50
24	BG	401	CLA	C1B-NB	-2.07	1.35	1.37
38	a	409	PHO	C3B-CAB	-2.07	1.43	1.47
31	2	404	PL9	C46-C44	-2.07	1.47	1.51
24	BQ	603	CLA	CMD-C2D	-2.07	1.46	1.50
24	y	312	CLA	CHC-C1C	2.07	1.42	1.38
23	Y	310	CHL	CHB-C4A	-2.07	1.32	1.37
24	d	401	CLA	CHC-C1C	2.07	1.42	1.38
23	AB	306	CHL	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	515	BCR	C38-C26	-2.07	1.47	1.50
24	G	611	CLA	CHC-C1C	2.07	1.42	1.38
24	BJ	614	CLA	CHC-C1C	2.07	1.42	1.38
23	5	607	CHL	C4C-C3C	2.07	1.48	1.45
24	1	503	CLA	C1B-NB	-2.07	1.35	1.37
24	C	507	CLA	MG-ND	-2.07	2.01	2.05
24	6	613	CLA	CMC-C2C	-2.07	1.46	1.50
24	C	511	CLA	CMC-C2C	-2.07	1.46	1.50
24	BV	610	CLA	CMD-C2D	-2.07	1.46	1.50
24	Ba	311	CLA	CMD-C2D	-2.07	1.46	1.50
34	C	518	DGD	O2G-C2G	-2.07	1.41	1.46
24	BF	510	CLA	MG-ND	-2.07	2.01	2.05
24	BE	608	CLA	CMB-C2B	-2.07	1.46	1.50
23	Au	609	CHL	CHB-C4A	-2.07	1.32	1.37
29	Ay	102	BCR	C33-C5	-2.07	1.47	1.50
24	y	315	CLA	CMB-C2B	-2.07	1.46	1.50
24	c	505	CLA	CMD-C2D	-2.07	1.46	1.50
23	5	609	CHL	C3B-C2B	2.07	1.48	1.41
24	AA	304	CLA	MG-ND	-2.07	2.01	2.05
24	7	305	CLA	CMD-C2D	-2.07	1.46	1.50
24	Y	305	CLA	CMD-C2D	-2.07	1.46	1.50
24	b	613	CLA	CMB-C2B	-2.07	1.46	1.50
24	BF	503	CLA	CMC-C2C	-2.07	1.46	1.50
24	n	602	CLA	MG-NB	-2.07	2.01	2.05
24	5	611	CLA	CMB-C2B	-2.07	1.46	1.50
24	s	609	CLA	CMC-C2C	-2.07	1.46	1.50
24	AA	311	CLA	CMB-C2B	-2.07	1.46	1.50
24	Ba	315	CLA	CMB-C2B	-2.07	1.46	1.50
32	BO	101	SQD	C8-C7	2.07	1.56	1.50
24	s	603	CLA	CMD-C2D	-2.07	1.46	1.50
24	a	405	CLA	MG-ND	-2.07	2.01	2.05
23	A2	606	CHL	CHB-C4A	-2.07	1.32	1.37
24	Y	312	CLA	CMC-C2C	-2.07	1.46	1.50
24	BJ	602	CLA	CMD-C2D	-2.07	1.46	1.50
24	BV	611	CLA	CMC-C2C	-2.07	1.46	1.50
23	BJ	601	CHL	C1B-NB	-2.07	1.35	1.37
24	S	604	CLA	CHC-C1C	2.07	1.42	1.38
23	Au	606	CHL	CHB-C4A	-2.07	1.32	1.37
29	1	515	BCR	C33-C5	-2.07	1.47	1.50
24	B	604	CLA	CMC-C2C	-2.07	1.46	1.50
24	S	604	CLA	CMC-C2C	-2.07	1.46	1.50
23	Au	606	CHL	C1B-C2B	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	CMC-C2C	-2.07	1.46	1.50
24	g	611	CLA	MG-NB	-2.07	2.01	2.05
24	7	314	CLA	CMB-C2B	-2.07	1.46	1.50
24	C	506	CLA	MG-ND	-2.07	2.01	2.05
24	B	614	CLA	CMC-C2C	-2.07	1.46	1.50
23	r	605	CHL	CHB-C4A	-2.07	1.32	1.37
24	C	503	CLA	MG-ND	-2.07	2.01	2.05
24	BE	617	CLA	CMB-C2B	-2.07	1.46	1.50
23	N	609	CHL	CHB-C4A	-2.07	1.32	1.37
24	A	407	CLA	C1B-NB	-2.07	1.35	1.37
25	9	616	LUT	C28-C29	-2.07	1.41	1.45
30	D	405	LMG	O7-C8	-2.07	1.41	1.46
24	s	609	CLA	CMD-C2D	-2.07	1.46	1.50
32	2	408	SQD	O7-S	2.07	1.51	1.45
24	AA	314	CLA	MG-ND	-2.07	2.01	2.05
23	6	609	CHL	C2C-C1C	2.07	1.49	1.44
24	BV	613	CLA	CMC-C2C	-2.07	1.46	1.50
24	1	509	CLA	C1B-NB	-2.07	1.35	1.37
24	BE	603	CLA	CHC-C1C	2.07	1.42	1.38
24	S	613	CLA	CMC-C2C	-2.07	1.46	1.50
24	9	603	CLA	CMD-C2D	-2.07	1.46	1.50
24	0	613	CLA	CMC-C2C	-2.07	1.46	1.50
24	v	614	CLA	CMC-C2C	-2.07	1.46	1.50
34	1	518	DGD	O2G-C2G	-2.06	1.41	1.46
24	B	601	CLA	CHC-C1C	2.06	1.42	1.38
24	BE	604	CLA	CMD-C2D	-2.06	1.46	1.50
23	G	606	CHL	C1D-ND	-2.06	1.35	1.37
24	s	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	9	611	CLA	CMB-C2B	-2.06	1.46	1.50
24	Au	610	CLA	CMC-C2C	-2.06	1.46	1.50
23	A2	607	CHL	C4C-C3C	2.06	1.48	1.45
24	1	502	CLA	CHC-C1C	2.06	1.42	1.38
29	1	515	BCR	C38-C26	-2.06	1.47	1.50
24	v	609	CLA	CMB-C2B	-2.06	1.46	1.50
24	8	308	CLA	C1A-CHA	-2.06	1.34	1.43
23	5	606	CHL	C1D-ND	-2.06	1.35	1.37
24	1	511	CLA	C1B-NB	-2.06	1.35	1.37
28	BJ	619	XAT	C38-C25	2.06	1.55	1.51
24	6	612	CLA	CMB-C2B	-2.06	1.46	1.50
24	n	603	CLA	CMB-C2B	-2.06	1.46	1.50
24	R	406	CLA	CHC-C1C	2.06	1.42	1.38
24	9	610	CLA	C1B-C2B	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	311	CLA	CMD-C2D	-2.06	1.46	1.50
24	N	614	CLA	CMD-C2D	-2.06	1.46	1.50
24	BQ	612	CLA	CHC-C1C	2.06	1.42	1.38
23	N	606	CHL	CHB-C4A	-2.06	1.32	1.37
24	v	612	CLA	C1B-NB	-2.06	1.35	1.37
23	Y	302	CHL	C4C-C3C	2.06	1.48	1.45
23	r	613	CHL	C4C-C3C	2.06	1.48	1.45
24	A2	610	CLA	CMC-C2C	-2.06	1.46	1.50
24	BQ	602	CLA	MG-NB	-2.06	2.01	2.05
29	BF	515	BCR	C33-C5	-2.06	1.47	1.50
28	7	318	XAT	C20-C13	2.06	1.55	1.50
24	A	406	CLA	C1B-NB	-2.06	1.35	1.37
24	8	310	CLA	CHC-C1C	2.06	1.42	1.38
24	n	611	CLA	MG-NB	-2.06	2.01	2.05
24	b	616	CLA	CMB-C2B	-2.06	1.46	1.50
24	BE	610	CLA	CMB-C2B	-2.06	1.46	1.50
24	BF	512	CLA	CMD-C2D	-2.06	1.46	1.50
23	BB	308	CHL	CHB-C4A	-2.06	1.32	1.37
29	BF	515	BCR	C38-C26	-2.06	1.47	1.50
24	Y	315	CLA	MG-ND	-2.06	2.01	2.05
33	f	102	HEM	CMB-C2B	2.06	1.55	1.50
29	Bb	101	BCR	C33-C5	-2.06	1.47	1.50
34	BD	413	DGD	O1G-C1G	-2.06	1.40	1.45
23	Au	605	CHL	C4B-NB	-2.06	1.35	1.37
24	r	614	CLA	CMB-C2B	-2.06	1.46	1.50
24	r	610	CLA	CMB-C2B	-2.06	1.46	1.50
24	AB	310	CLA	CMD-C2D	-2.06	1.46	1.50
24	A6	603	CLA	CMC-C2C	-2.06	1.46	1.50
26	g	617	NEX	C32-C33	-2.06	1.41	1.45
24	7	311	CLA	CHC-C1C	2.06	1.42	1.38
24	BV	610	CLA	CHC-C1C	2.06	1.42	1.38
34	1	516	DGD	O5D-C6D	-2.06	1.40	1.43
24	G	612	CLA	CMB-C2B	-2.06	1.46	1.50
24	b	610	CLA	CMB-C2B	-2.06	1.46	1.50
24	BD	410	CLA	CMC-C2C	-2.06	1.46	1.50
26	Ba	318	NEX	C12-C13	-2.06	1.41	1.45
23	Ba	308	CHL	CHB-C4A	-2.06	1.32	1.37
23	S	605	CHL	MG-NA	-2.06	2.01	2.06
24	g	612	CLA	MG-NB	-2.06	2.01	2.05
24	c	510	CLA	MG-ND	-2.06	2.01	2.05
24	S	602	CLA	CHC-C1C	2.06	1.42	1.38
24	c	514	CLA	MG-ND	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	CMB-C2B	-2.06	1.46	1.50
24	AA	311	CLA	CMD-C2D	-2.06	1.46	1.50
38	A	409	PHO	C3D-C4D	2.06	1.44	1.41
24	BF	511	CLA	MG-ND	-2.06	2.01	2.05
24	B	601	CLA	CMD-C2D	-2.06	1.46	1.50
24	G	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	S	608	CLA	CMD-C2D	-2.06	1.46	1.50
24	s	608	CLA	CMD-C2D	-2.06	1.46	1.50
24	Au	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	5	614	CLA	CMB-C2B	-2.06	1.46	1.50
24	A	406	CLA	CMC-C2C	-2.06	1.46	1.50
24	y	305	CLA	CMD-C2D	-2.06	1.46	1.50
24	9	614	CLA	CMB-C2B	-2.06	1.46	1.50
24	0	603	CLA	CMC-C2C	-2.06	1.46	1.50
24	AA	315	CLA	CMD-C2D	-2.06	1.46	1.50
24	BU	601	CLA	C1B-NB	-2.06	1.35	1.37
29	BN	101	BCR	C33-C5	-2.06	1.47	1.50
34	R	401	DGD	O1G-C1G	-2.06	1.40	1.45
24	6	611	CLA	MG-ND	-2.06	2.01	2.05
24	2	403	CLA	CHC-C1C	2.05	1.42	1.38
24	G	610	CLA	CMC-C2C	-2.05	1.46	1.50
24	BV	611	CLA	CMD-C2D	-2.05	1.46	1.50
24	Ba	304	CLA	CMB-C2B	-2.05	1.46	1.50
23	N	601	CHL	C1D-ND	-2.05	1.35	1.37
24	s	611	CLA	CHC-C1C	2.05	1.42	1.38
24	Au	611	CLA	CHC-C1C	2.05	1.42	1.38
28	AA	301	XAT	C24-C25	2.05	1.55	1.52
23	Ba	308	CHL	MG-NA	-2.05	2.01	2.06
23	Y	307	CHL	C4B-NB	-2.05	1.35	1.37
24	5	613	CLA	CMC-C2C	-2.05	1.46	1.50
24	BE	616	CLA	CMB-C2B	-2.05	1.46	1.50
24	R	406	CLA	CMC-C2C	-2.05	1.46	1.50
23	BJ	608	CHL	MG-NA	-2.05	2.01	2.06
23	BV	606	CHL	C1B-NB	-2.05	1.35	1.37
32	l	102	SQD	O9-S	2.05	1.51	1.45
24	v	605	CLA	CHC-C1C	2.05	1.42	1.38
24	y	311	CLA	CMD-C2D	-2.05	1.46	1.50
24	BV	604	CLA	CMD-C2D	-2.05	1.46	1.50
23	g	605	CHL	MG-NA	-2.05	2.01	2.06
24	BE	616	CLA	CHC-C1C	2.05	1.42	1.38
24	s	610	CLA	CMD-C2D	-2.05	1.46	1.50
30	C	519	LMG	O7-C8	-2.05	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	615	LUT	C32-C33	-2.05	1.41	1.45
24	b	605	CLA	CMC-C2C	-2.05	1.46	1.50
24	c	512	CLA	CMC-C2C	-2.05	1.46	1.50
24	N	604	CLA	C1B-NB	-2.05	1.35	1.37
24	s	611	CLA	CMC-C2C	-2.05	1.46	1.50
24	BE	609	CLA	CMC-C2C	-2.05	1.46	1.50
23	8	304	CHL	C4C-C3C	2.05	1.48	1.45
23	N	605	CHL	C4C-C3C	2.05	1.48	1.45
23	Au	607	CHL	CHB-C4A	-2.05	1.32	1.37
24	B	601	CLA	CMB-C2B	-2.05	1.46	1.50
24	b	615	CLA	CMC-C2C	-2.05	1.46	1.50
24	v	609	CLA	CMC-C2C	-2.05	1.46	1.50
24	BQ	612	CLA	CMD-C2D	-2.05	1.46	1.50
23	Au	601	CHL	C4C-C3C	2.05	1.48	1.45
23	6	609	CHL	MG-ND	-2.05	2.01	2.05
24	BE	607	CLA	CHC-C1C	2.05	1.42	1.38
24	BV	611	CLA	CHC-C1C	2.05	1.42	1.38
24	d	401	CLA	MG-ND	-2.05	2.01	2.05
23	7	308	CHL	C4C-C3C	2.05	1.48	1.45
23	BB	307	CHL	C1B-C2B	2.05	1.48	1.43
31	2	404	PL9	C31-C29	-2.05	1.47	1.51
32	l	101	SQD	C8-C7	2.05	1.56	1.50
30	BL	101	LMG	O7-C8	-2.05	1.41	1.46
24	2	403	CLA	CMB-C2B	-2.05	1.46	1.50
24	BF	505	CLA	CMB-C2B	-2.05	1.46	1.50
24	B	615	CLA	CHC-C1C	2.05	1.42	1.38
24	BE	611	CLA	CHC-C1C	2.05	1.42	1.38
23	A2	608	CHL	CHB-C4A	-2.05	1.32	1.37
24	B	602	CLA	CMC-C2C	-2.05	1.46	1.50
24	BV	602	CLA	CMB-C2B	-2.05	1.46	1.50
24	BV	610	CLA	CMB-C2B	-2.05	1.46	1.50
24	BF	509	CLA	CMC-C2C	-2.05	1.46	1.50
34	1	516	DGD	O4E-C4E	-2.05	1.38	1.43
24	BV	603	CLA	CMD-C2D	-2.05	1.46	1.50
24	BU	610	CLA	CMB-C2B	-2.05	1.46	1.50
26	S	616	NEX	C12-C13	-2.05	1.41	1.45
24	7	311	CLA	CMB-C2B	-2.05	1.46	1.50
24	7	312	CLA	CHC-C1C	2.05	1.42	1.38
24	BE	610	CLA	CHC-C1C	2.05	1.42	1.38
23	Au	607	CHL	C4C-C3C	2.05	1.48	1.45
24	B	606	CLA	CHC-C1C	2.05	1.42	1.38
24	S	612	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	CMC-C2C	-2.05	1.46	1.50
28	Ba	301	XAT	C38-C25	2.05	1.55	1.51
24	BV	609	CLA	MG-NB	-2.05	2.01	2.05
24	BG	401	CLA	MG-ND	-2.05	2.01	2.05
24	D	402	CLA	CMB-C2B	-2.05	1.46	1.50
24	b	610	CLA	CMD-C2D	-2.05	1.46	1.50
24	0	610	CLA	CHC-C1C	2.04	1.42	1.38
24	BQ	604	CLA	CHC-C1C	2.04	1.42	1.38
28	AA	318	XAT	C20-C13	2.04	1.55	1.50
24	n	613	CLA	CMC-C2C	-2.04	1.46	1.50
24	BE	610	CLA	CMD-C2D	-2.04	1.46	1.50
24	1	503	CLA	MG-ND	-2.04	2.01	2.05
29	c	515	BCR	C33-C5	-2.04	1.47	1.50
23	N	608	CHL	CHB-C4A	-2.04	1.32	1.37
23	y	308	CHL	MG-NA	-2.04	2.01	2.06
24	B	607	CLA	CHC-C1C	2.04	1.42	1.38
24	B	608	CLA	CMD-C2D	-2.04	1.46	1.50
24	s	602	CLA	CMB-C2B	-2.04	1.46	1.50
24	0	614	CLA	CMC-C2C	-2.04	1.46	1.50
24	v	615	CLA	CMC-C2C	-2.04	1.46	1.50
27	BY	201	LHG	O7-C5	-2.04	1.41	1.46
24	BF	514	CLA	MG-ND	-2.04	2.01	2.05
24	C	502	CLA	CHC-C1C	2.04	1.42	1.38
24	BE	615	CLA	CHC-C1C	2.04	1.42	1.38
24	BE	605	CLA	CMC-C2C	-2.04	1.46	1.50
30	i	101	LMG	O7-C8	-2.04	1.41	1.46
23	A6	605	CHL	C1D-ND	-2.04	1.35	1.37
24	R	405	CLA	C1B-NB	-2.04	1.35	1.37
24	8	303	CLA	CMC-C2C	-2.04	1.46	1.50
24	c	506	CLA	CMC-C2C	-2.04	1.46	1.50
24	0	603	CLA	CHC-C1C	2.04	1.42	1.38
24	v	610	CLA	CHC-C1C	2.04	1.42	1.38
24	6	611	CLA	CMD-C2D	-2.04	1.46	1.50
33	BI	102	HEM	FE-NC	2.04	2.02	1.95
23	e	601	CHL	C4B-NB	-2.04	1.35	1.37
23	g	609	CHL	C1D-ND	-2.04	1.35	1.37
24	c	503	CLA	CMC-C2C	-2.04	1.46	1.50
24	AB	303	CLA	CMC-C2C	-2.04	1.46	1.50
24	BE	611	CLA	CMC-C2C	-2.04	1.46	1.50
38	A	409	PHO	C3B-CAB	-2.04	1.43	1.47
24	g	604	CLA	CMB-C2B	-2.04	1.46	1.50
24	BV	608	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BJ	607	CHL	C1B-NB	-2.04	1.35	1.37
24	b	608	CLA	CMC-C2C	-2.04	1.46	1.50
24	AA	314	CLA	CMB-C2B	-2.04	1.46	1.50
24	BE	608	CLA	CMC-C2C	-2.04	1.46	1.50
24	Ba	305	CLA	CMD-C2D	-2.04	1.46	1.50
28	g	619	XAT	C38-C25	2.04	1.55	1.51
24	BF	512	CLA	CMC-C2C	-2.04	1.46	1.50
24	Au	610	CLA	CHC-C1C	2.04	1.42	1.38
24	BJ	604	CLA	CMB-C2B	-2.04	1.46	1.50
24	BB	313	CLA	C1B-NB	-2.04	1.35	1.37
24	y	305	CLA	CMB-C2B	-2.04	1.46	1.50
24	BJ	612	CLA	CMB-C2B	-2.04	1.46	1.50
29	C	515	BCR	C33-C5	-2.04	1.47	1.50
23	N	607	CHL	CHB-C4A	-2.04	1.32	1.37
23	A2	601	CHL	CHB-C4A	-2.04	1.32	1.37
24	0	611	CLA	CMD-C2D	-2.04	1.46	1.50
24	6	610	CLA	MG-ND	-2.04	2.01	2.05
24	n	604	CLA	CHC-C1C	2.04	1.42	1.38
32	BO	102	SQD	O9-S	2.04	1.51	1.45
24	BF	507	CLA	MG-ND	-2.04	2.01	2.05
24	B	607	CLA	CMB-C2B	-2.04	1.46	1.50
24	Ba	314	CLA	CMD-C2D	-2.04	1.46	1.50
24	5	610	CLA	C1B-C2B	2.04	1.48	1.43
23	BU	605	CHL	CHB-C4A	-2.04	1.32	1.37
24	C	508	CLA	MG-ND	-2.04	2.01	2.05
24	AA	304	CLA	CMD-C2D	-2.04	1.46	1.50
24	A2	610	CLA	CMD-C2D	-2.04	1.46	1.50
24	BE	606	CLA	CMC-C2C	-2.04	1.46	1.50
28	Ba	301	XAT	C20-C13	2.04	1.55	1.50
23	A2	607	CHL	CHB-C4A	-2.04	1.32	1.37
23	n	609	CHL	C4B-NB	-2.04	1.35	1.37
25	6	615	LUT	C35-C34	-2.04	1.37	1.43
24	B	611	CLA	CHC-C1C	2.04	1.42	1.38
29	BI	101	BCR	C33-C5	-2.04	1.47	1.50
24	s	604	CLA	CMB-C2B	-2.04	1.46	1.50
24	0	604	CLA	CMC-C2C	-2.04	1.46	1.50
24	1	513	CLA	CMC-C2C	-2.04	1.46	1.50
23	A2	601	CHL	C4C-C3C	2.04	1.48	1.45
24	c	511	CLA	MG-ND	-2.04	2.01	2.05
24	6	603	CLA	CHC-C1C	2.04	1.42	1.38
23	A6	605	CHL	CHB-C4A	-2.04	1.32	1.37
24	Y	305	CLA	MG-ND	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	CMC-C2C	-2.03	1.46	1.50
24	AA	305	CLA	CMD-C2D	-2.03	1.46	1.50
24	Ba	303	CLA	CMB-C2B	-2.03	1.46	1.50
24	1	512	CLA	C1B-NB	-2.03	1.35	1.37
24	8	308	CLA	CMB-C2B	-2.03	1.46	1.50
24	B	609	CLA	CHC-C1C	2.03	1.42	1.38
24	D	402	CLA	CHC-C1C	2.03	1.42	1.38
24	n	610	CLA	CHC-C1C	2.03	1.42	1.38
24	1	510	CLA	C1B-NB	-2.03	1.35	1.37
24	C	509	CLA	MG-ND	-2.03	2.01	2.05
24	1	509	CLA	MG-ND	-2.03	2.01	2.05
24	BF	512	CLA	MG-ND	-2.03	2.01	2.05
24	S	610	CLA	CMC-C2C	-2.03	1.46	1.50
24	n	604	CLA	CMD-C2D	-2.03	1.46	1.50
33	F	102	HEM	CMB-C2B	2.03	1.55	1.50
33	BI	102	HEM	CMC-C2C	2.03	1.55	1.50
23	7	302	CHL	CHB-C4A	-2.03	1.32	1.37
26	7	319	NEX	C11-C12	2.03	1.39	1.34
24	A6	611	CLA	MG-ND	-2.03	2.01	2.05
24	5	603	CLA	CMD-C2D	-2.03	1.46	1.50
23	e	601	CHL	MG-NA	-2.03	2.01	2.06
23	A6	601	CHL	C4B-NB	-2.03	1.35	1.37
30	1	519	LMG	O7-C8	-2.03	1.41	1.46
24	B	608	CLA	CMC-C2C	-2.03	1.46	1.50
23	A6	605	CHL	MG-NA	-2.03	2.01	2.06
29	F	101	BCR	C33-C5	-2.03	1.47	1.50
24	y	315	CLA	CHC-C1C	2.03	1.42	1.38
24	B	606	CLA	CMC-C2C	-2.03	1.46	1.50
24	AA	305	CLA	CMB-C2B	-2.03	1.46	1.50
24	BJ	612	CLA	MG-NB	-2.03	2.01	2.05
24	Aw	102	CLA	C1B-NB	-2.03	1.35	1.37
24	G	610	CLA	CHC-C1C	2.03	1.42	1.38
24	Ba	312	CLA	CHC-C1C	2.03	1.42	1.38
24	c	513	CLA	MG-ND	-2.03	2.01	2.05
24	A6	602	CLA	CHC-C1C	2.03	1.42	1.38
24	s	612	CLA	CMD-C2D	-2.03	1.46	1.50
24	BE	607	CLA	CMD-C2D	-2.03	1.46	1.50
24	R	409	CLA	CMC-C2C	-2.03	1.46	1.50
23	BV	605	CHL	MG-NA	-2.03	2.01	2.06
24	BB	314	CLA	C1B-NB	-2.03	1.35	1.37
24	1	508	CLA	C1B-NB	-2.03	1.35	1.37
23	BU	613	CHL	C4C-C3C	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	312	CLA	CMD-C2D	-2.03	1.46	1.50
24	A6	608	CLA	CMB-C2B	-2.03	1.46	1.50
24	c	512	CLA	CHC-C1C	2.03	1.42	1.38
24	y	305	CLA	CMC-C2C	-2.03	1.46	1.50
24	A2	602	CLA	CHC-C1C	2.03	1.42	1.38
24	C	512	CLA	MG-ND	-2.03	2.01	2.05
24	BE	614	CLA	MG-ND	-2.03	2.01	2.05
23	y	307	CHL	C1D-ND	-2.03	1.35	1.37
24	Ba	303	CLA	CMD-C2D	-2.03	1.46	1.50
24	C	506	CLA	CHC-C1C	2.03	1.42	1.38
24	Y	304	CLA	CMC-C2C	-2.03	1.46	1.50
24	9	610	CLA	CMC-C2C	-2.03	1.46	1.50
24	A2	614	CLA	CMB-C2B	-2.03	1.46	1.50
23	Ba	310	CHL	C3B-C2B	2.03	1.48	1.41
24	7	305	CLA	CMB-C2B	-2.03	1.46	1.50
24	b	608	CLA	CMB-C2B	-2.03	1.46	1.50
24	BE	612	CLA	CHC-C1C	2.03	1.42	1.38
28	y	301	XAT	C20-C13	2.03	1.55	1.50
28	Au	619	XAT	C20-C13	2.03	1.55	1.50
28	BJ	619	XAT	C20-C13	2.03	1.55	1.50
24	7	311	CLA	CBD-CGD	-2.03	1.49	1.51
24	BB	312	CLA	MG-ND	-2.03	2.01	2.05
24	7	313	CLA	CHC-C1C	2.03	1.42	1.38
24	C	512	CLA	CHC-C1C	2.03	1.42	1.38
29	K	102	BCR	C33-C5	-2.03	1.47	1.50
24	S	603	CLA	CMB-C2B	-2.03	1.46	1.50
24	A6	603	CLA	CMB-C2B	-2.03	1.46	1.50
23	7	302	CHL	C1D-ND	-2.03	1.35	1.37
24	B	605	CLA	CHC-C1C	2.03	1.42	1.38
24	v	609	CLA	CHC-C1C	2.03	1.42	1.38
24	A6	610	CLA	CHC-C1C	2.03	1.42	1.38
24	6	603	CLA	CMC-C2C	-2.02	1.46	1.50
24	a	410	CLA	CMC-C2C	-2.02	1.46	1.50
24	y	305	CLA	CHC-C1C	2.02	1.42	1.38
24	1	506	CLA	C1B-NB	-2.02	1.35	1.37
27	C	521	LHG	O7-C5	-2.02	1.41	1.46
23	9	609	CHL	MG-ND	-2.02	2.01	2.05
31	D	403	PL9	C46-C44	-2.02	1.47	1.51
23	n	606	CHL	C1D-ND	-2.02	1.35	1.37
24	B	613	CLA	CMC-C2C	-2.02	1.46	1.50
24	BQ	603	CLA	CMB-C2B	-2.02	1.46	1.50
24	s	609	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	304	CLA	MG-ND	-2.02	2.01	2.05
28	BQ	619	XAT	C38-C25	2.02	1.55	1.51
28	G	619	XAT	C20-C13	2.02	1.55	1.50
29	1	514	BCR	C38-C26	-2.02	1.47	1.50
23	BH	601	CHL	MG-NA	-2.02	2.01	2.06
23	AA	306	CHL	C2C-C1C	2.02	1.48	1.44
24	b	609	CLA	CMC-C2C	-2.02	1.46	1.50
24	Y	303	CLA	CHC-C1C	2.02	1.42	1.38
24	Ba	315	CLA	CHC-C1C	2.02	1.42	1.38
24	c	514	CLA	C1B-NB	-2.02	1.35	1.37
29	1	514	BCR	C33-C5	-2.02	1.47	1.50
24	Au	603	CLA	CHC-C1C	2.02	1.42	1.38
24	AA	313	CLA	CMB-C2B	-2.02	1.46	1.50
24	B	609	CLA	CMC-C2C	-2.02	1.46	1.50
24	A6	613	CLA	CMC-C2C	-2.02	1.46	1.50
24	v	611	CLA	CHC-C1C	2.02	1.42	1.38
24	Y	312	CLA	MG-ND	-2.02	2.01	2.05
24	BE	602	CLA	CMC-C2C	-2.02	1.46	1.50
23	G	605	CHL	C4B-NB	-2.02	1.35	1.37
24	BE	604	CLA	CHC-C1C	2.02	1.42	1.38
24	s	603	CLA	MG-NB	-2.02	2.01	2.05
24	A	405	CLA	MG-ND	-2.02	2.01	2.05
38	BD	409	PHO	C3D-C4D	2.02	1.44	1.41
24	s	604	CLA	CMC-C2C	-2.02	1.46	1.50
24	s	611	CLA	CMD-C2D	-2.02	1.46	1.50
24	y	314	CLA	CMD-C2D	-2.02	1.46	1.50
23	S	601	CHL	CHB-C4A	-2.02	1.32	1.37
23	BJ	609	CHL	C2C-C1C	2.02	1.48	1.44
24	G	603	CLA	CMC-C2C	-2.02	1.46	1.50
24	b	607	CLA	CMD-C2D	-2.02	1.46	1.50
24	AB	308	CLA	C1B-NB	-2.02	1.35	1.37
23	n	606	CHL	C2C-C1C	2.02	1.48	1.44
23	AA	302	CHL	CHB-C4A	-2.02	1.32	1.37
24	1	510	CLA	MG-ND	-2.02	2.01	2.05
24	9	604	CLA	CMC-C2C	-2.02	1.46	1.50
24	BE	616	CLA	CMC-C2C	-2.02	1.46	1.50
24	BV	612	CLA	CMD-C2D	-2.02	1.46	1.50
24	BF	506	CLA	CMC-C2C	-2.02	1.46	1.50
23	s	606	CHL	C2C-C1C	2.02	1.48	1.44
23	BQ	607	CHL	CHB-C4A	-2.02	1.32	1.37
24	AB	310	CLA	CHC-C1C	2.02	1.42	1.38
24	1	504	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	406	CLA	MG-ND	-2.02	2.01	2.05
29	z	102	BCR	C33-C5	-2.02	1.47	1.50
32	2	408	SQD	C46-C45	2.02	1.56	1.50
23	BJ	607	CHL	C4B-NB	-2.02	1.35	1.37
23	Ba	310	CHL	C1B-NB	-2.02	1.35	1.37
24	8	309	CLA	CMD-C2D	-2.02	1.46	1.50
28	g	619	XAT	C20-C13	2.02	1.55	1.50
23	g	606	CHL	C4D-CHA	2.02	1.45	1.38
28	G	619	XAT	C38-C25	2.02	1.55	1.51
24	y	304	CLA	CMB-C2B	-2.02	1.46	1.50
24	BV	612	CLA	CHC-C1C	2.02	1.42	1.38
23	BB	309	CHL	CHB-C4A	-2.02	1.32	1.37
24	S	603	CLA	CMC-C2C	-2.02	1.46	1.50
24	s	610	CLA	CHC-C1C	2.02	1.42	1.38
24	c	514	CLA	CHC-C1C	2.02	1.42	1.38
24	1	504	CLA	MG-ND	-2.02	2.01	2.05
24	g	613	CLA	CMD-C2D	-2.02	1.46	1.50
24	BQ	613	CLA	CMC-C2C	-2.02	1.46	1.50
23	N	601	CHL	CHB-C4A	-2.02	1.32	1.37
24	BD	405	CLA	MG-ND	-2.02	2.01	2.05
24	0	602	CLA	CMD-C2D	-2.02	1.46	1.50
24	BE	603	CLA	CMC-C2C	-2.02	1.46	1.50
28	Y	301	XAT	C38-C25	2.02	1.55	1.51
24	y	303	CLA	CMB-C2B	-2.02	1.46	1.50
24	v	606	CLA	CMC-C2C	-2.01	1.46	1.50
27	BF	521	LHG	O7-C5	-2.01	1.41	1.46
27	5	618	LHG	O7-C5	-2.01	1.41	1.46
24	7	312	CLA	CMD-C2D	-2.01	1.46	1.50
24	Au	614	CLA	CMD-C2D	-2.01	1.46	1.50
23	g	601	CHL	MG-NA	-2.01	2.01	2.06
23	BJ	601	CHL	MG-NA	-2.01	2.01	2.06
24	c	505	CLA	CMB-C2B	-2.01	1.46	1.50
24	BF	504	CLA	CMC-C2C	-2.01	1.46	1.50
23	BJ	606	CHL	C4D-CHA	2.01	1.45	1.38
24	5	602	CLA	CMD-C2D	-2.01	1.46	1.50
24	n	612	CLA	CMD-C2D	-2.01	1.46	1.50
24	s	612	CLA	CHC-C1C	2.01	1.42	1.38
24	1	506	CLA	CHC-C1C	2.01	1.42	1.38
29	f	101	BCR	C33-C5	-2.01	1.47	1.50
24	Y	304	CLA	MG-ND	-2.01	2.01	2.05
24	b	606	CLA	CMC-C2C	-2.01	1.46	1.50
24	8	302	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	604	CLA	CMC-C2C	-2.01	1.46	1.50
24	B	610	CLA	CHC-C1C	2.01	1.42	1.38
23	Au	607	CHL	C4B-NB	-2.01	1.35	1.37
24	S	610	CLA	CHC-C1C	2.01	1.42	1.38
23	A6	601	CHL	CHB-C4A	-2.01	1.32	1.37
23	g	608	CHL	MG-NA	-2.01	2.01	2.06
24	n	613	CLA	CMB-C2B	-2.01	1.46	1.50
24	9	613	CLA	CMB-C2B	-2.01	1.46	1.50
24	BQ	613	CLA	CMB-C2B	-2.01	1.46	1.50
23	BQ	609	CHL	C2C-C1C	2.01	1.48	1.44
29	z	101	BCR	C38-C26	-2.01	1.47	1.50
23	Ba	307	CHL	C1D-ND	-2.01	1.35	1.37
24	BB	304	CLA	C1B-NB	-2.01	1.35	1.37
24	C	513	CLA	CHC-C1C	2.01	1.42	1.38
24	b	603	CLA	CMC-C2C	-2.01	1.46	1.50
24	A	407	CLA	CMC-C2C	-2.01	1.46	1.50
24	BQ	603	CLA	CMC-C2C	-2.01	1.46	1.50
23	BB	309	CHL	C4B-NB	-2.01	1.35	1.37
23	n	607	CHL	CHB-C4A	-2.01	1.32	1.37
24	BB	312	CLA	CHC-C1C	2.01	1.42	1.38
28	n	619	XAT	C38-C25	2.01	1.55	1.51
24	b	610	CLA	CHC-C1C	2.01	1.42	1.38
24	d	402	CLA	CHC-C1C	2.01	1.42	1.38
24	G	614	CLA	CMD-C2D	-2.01	1.46	1.50
24	0	612	CLA	CMB-C2B	-2.01	1.46	1.50
24	8	310	CLA	CMD-C2D	-2.01	1.46	1.50
24	AA	305	CLA	CMC-C2C	-2.01	1.46	1.50
24	b	613	CLA	CHC-C1C	2.01	1.42	1.38
24	b	615	CLA	CHC-C1C	2.01	1.42	1.38
24	g	611	CLA	CMB-C2B	-2.01	1.46	1.50
24	s	613	CLA	CMC-C2C	-2.01	1.46	1.50
24	S	608	CLA	CMB-C2B	-2.01	1.46	1.50
24	g	610	CLA	CMD-C2D	-2.01	1.46	1.50
24	Y	313	CLA	C1B-NB	-2.01	1.35	1.37
24	8	309	CLA	MG-ND	-2.01	2.01	2.05
24	G	602	CLA	CHC-C1C	2.01	1.42	1.38
24	BQ	613	CLA	CHC-C1C	2.01	1.42	1.38
24	5	610	CLA	CMC-C2C	-2.01	1.46	1.50
24	BE	613	CLA	CHC-C1C	2.01	1.42	1.38
29	Ay	102	BCR	C38-C26	-2.01	1.47	1.50
23	BJ	606	CHL	CHB-C4A	-2.01	1.32	1.37
24	5	614	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	604	CLA	CMD-C2D	-2.01	1.46	1.50
24	7	313	CLA	CMB-C2B	-2.01	1.46	1.50
24	BQ	604	CLA	CMD-C2D	-2.01	1.46	1.50
24	BV	604	CLA	MG-ND	-2.01	2.01	2.05
25	5	616	LUT	C28-C29	-2.01	1.41	1.45
24	7	314	CLA	CMC-C2C	-2.01	1.46	1.50
24	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
24	R	404	CLA	MG-ND	-2.01	2.01	2.05
32	Az	101	SQD	O9-S	2.01	1.50	1.45
24	b	616	CLA	CMC-C2C	-2.01	1.46	1.50
24	c	504	CLA	CMC-C2C	-2.01	1.46	1.50
24	9	602	CLA	CMD-C2D	-2.01	1.46	1.50
23	BQ	606	CHL	C1D-ND	-2.01	1.35	1.37
23	N	608	CHL	C4C-C3C	2.00	1.48	1.45
24	c	505	CLA	CMC-C2C	-2.00	1.46	1.50
26	G	617	NEX	C11-C12	2.00	1.39	1.34
24	y	303	CLA	CMD-C2D	-2.00	1.46	1.50
24	BV	604	CLA	C1B-C2B	2.00	1.48	1.43
24	N	603	CLA	CHC-C1C	2.00	1.42	1.38
24	BU	604	CLA	CMC-C2C	-2.00	1.46	1.50
24	S	611	CLA	CHC-C1C	2.00	1.42	1.38
24	Y	304	CLA	CHC-C1C	2.00	1.42	1.38
24	a	407	CLA	CHC-C1C	2.00	1.42	1.38
24	BF	514	CLA	CHC-C1C	2.00	1.42	1.38
23	BJ	609	CHL	CMC-C2C	2.00	1.49	1.45
24	r	612	CLA	C1B-NB	-2.00	1.35	1.37
32	L	103	SQD	C8-C7	2.00	1.56	1.50
24	6	614	CLA	CMC-C2C	-2.00	1.46	1.50
24	g	602	CLA	CMD-C2D	-2.00	1.46	1.50
24	BD	407	CLA	CMC-C2C	-2.00	1.46	1.50
23	y	308	CHL	CHB-C4A	-2.00	1.32	1.37
24	5	612	CLA	CHC-C1C	2.00	1.42	1.38
24	b	607	CLA	CHC-C1C	2.00	1.42	1.38
24	a	407	CLA	CMC-C2C	-2.00	1.46	1.50
24	R	406	CLA	C1B-NB	-2.00	1.35	1.37
24	A6	613	CLA	CHC-C1C	2.00	1.42	1.38
24	B	615	CLA	CMC-C2C	-2.00	1.46	1.50
24	g	603	CLA	CMB-C2B	-2.00	1.46	1.50
24	7	304	CLA	MG-ND	-2.00	2.01	2.05
24	BF	507	CLA	CHC-C1C	2.00	1.42	1.38
24	BJ	611	CLA	CMB-C2B	-2.00	1.46	1.50
24	8	301	CLA	CHC-C1C	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	CMC-C2C	-2.00	1.46	1.50
29	z	101	BCR	C33-C5	-2.00	1.47	1.50
24	c	511	CLA	C1B-NB	-2.00	1.35	1.37
24	Ba	305	CLA	CMC-C2C	-2.00	1.46	1.50
24	Y	311	CLA	MG-ND	-2.00	2.01	2.05
24	c	507	CLA	MG-ND	-2.00	2.01	2.05
23	Y	309	CHL	CHB-C4A	-2.00	1.32	1.37
24	7	304	CLA	CMD-C2D	-2.00	1.46	1.50
24	s	610	CLA	CMB-C2B	-2.00	1.46	1.50

All (8154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BB	301	XAT	O24-C25-C24	33.02	138.19	113.38
28	AA	301	XAT	O24-C25-C24	32.93	138.12	113.38
28	N	619	XAT	O24-C25-C24	32.85	138.06	113.38
28	5	619	XAT	O4-C5-C4	32.85	138.06	113.38
28	A2	619	XAT	O24-C25-C24	32.82	138.04	113.38
28	9	619	XAT	O4-C5-C4	32.72	137.96	113.38
28	Y	301	XAT	O24-C25-C24	32.69	137.94	113.38
28	7	301	XAT	O24-C25-C24	32.67	137.92	113.38
28	AA	318	XAT	O24-C25-C24	32.55	137.84	113.38
28	7	318	XAT	O24-C25-C24	32.43	137.75	113.38
28	BB	301	XAT	O4-C5-C4	32.41	137.73	113.38
28	Y	301	XAT	O4-C5-C4	32.33	137.67	113.38
28	Au	619	XAT	O24-C25-C24	32.31	137.65	113.38
28	y	301	XAT	O24-C25-C24	32.30	137.65	113.38
28	G	619	XAT	O24-C25-C24	32.27	137.62	113.38
28	BQ	619	XAT	O4-C5-C4	32.25	137.60	113.38
28	Ba	301	XAT	O24-C25-C24	32.21	137.58	113.38
28	n	619	XAT	O4-C5-C4	32.04	137.45	113.38
28	g	619	XAT	O24-C25-C24	32.03	137.45	113.38
28	G	619	XAT	O4-C5-C4	32.01	137.43	113.38
28	Au	619	XAT	O4-C5-C4	32.01	137.43	113.38
28	BJ	619	XAT	O24-C25-C24	32.01	137.43	113.38
28	Ba	301	XAT	O4-C5-C4	31.98	137.40	113.38
28	8	312	XAT	O4-C5-C4	31.87	137.32	113.38
28	AB	312	XAT	O4-C5-C4	31.86	137.32	113.38
28	AA	318	XAT	O4-C5-C4	31.83	137.29	113.38
28	BQ	619	XAT	O24-C25-C24	31.82	137.28	113.38
28	7	318	XAT	O4-C5-C4	31.82	137.28	113.38
28	y	301	XAT	O4-C5-C4	31.76	137.24	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	AA	301	XAT	O4-C5-C4	31.74	137.23	113.38
28	g	619	XAT	O4-C5-C4	31.72	137.21	113.38
28	7	301	XAT	O4-C5-C4	31.70	137.20	113.38
28	n	619	XAT	O24-C25-C24	31.70	137.19	113.38
28	N	619	XAT	O4-C5-C4	31.67	137.17	113.38
28	BJ	619	XAT	O4-C5-C4	31.63	137.15	113.38
28	A2	619	XAT	O4-C5-C4	31.60	137.12	113.38
28	AB	312	XAT	O24-C25-C24	31.59	137.11	113.38
28	8	312	XAT	O24-C25-C24	31.54	137.08	113.38
28	r	616	XAT	O4-C5-C4	31.37	136.95	113.38
28	BU	616	XAT	O4-C5-C4	31.32	136.91	113.38
28	r	616	XAT	O24-C25-C24	30.98	136.65	113.38
28	BU	616	XAT	O24-C25-C24	30.87	136.57	113.38
28	5	619	XAT	O24-C25-C24	27.60	134.11	113.38
28	9	619	XAT	O24-C25-C24	27.54	134.07	113.38
23	g	607	CHL	C2B-C1B-NB	10.62	117.35	110.23
23	BJ	607	CHL	C2B-C1B-NB	10.58	117.32	110.23
28	AA	318	XAT	C31-C30-C29	-10.47	112.36	127.31
28	7	318	XAT	C31-C30-C29	-10.46	112.39	127.31
28	Ba	301	XAT	C15-C14-C13	-10.44	112.42	127.31
28	y	301	XAT	C15-C14-C13	-10.43	112.42	127.31
28	5	619	XAT	C11-C10-C9	-10.43	112.43	127.31
23	Ba	308	CHL	C2B-C1B-NB	10.38	117.19	110.23
23	5	606	CHL	C2B-C1B-NB	10.38	117.19	110.23
28	9	619	XAT	C31-C30-C29	-10.37	112.50	127.31
23	y	308	CHL	C2B-C1B-NB	10.37	117.19	110.23
23	AA	308	CHL	C2B-C1B-NB	10.34	117.17	110.23
28	5	619	XAT	C15-C14-C13	-10.34	112.55	127.31
28	A2	619	XAT	C15-C14-C13	-10.32	112.58	127.31
28	9	619	XAT	C35-C34-C33	-10.30	112.61	127.31
23	7	308	CHL	C2B-C1B-NB	10.29	117.13	110.23
28	AA	301	XAT	C15-C14-C13	-10.27	112.65	127.31
28	AA	318	XAT	C15-C14-C13	-10.26	112.66	127.31
23	G	607	CHL	C2B-C1B-NB	10.26	117.11	110.23
23	n	607	CHL	C2B-C1B-NB	10.25	117.10	110.23
28	N	619	XAT	C15-C14-C13	-10.25	112.68	127.31
23	BQ	607	CHL	C2B-C1B-NB	10.24	117.10	110.23
28	7	301	XAT	C15-C14-C13	-10.24	112.70	127.31
23	BJ	601	CHL	C2B-C1B-NB	10.22	117.08	110.23
23	0	606	CHL	C2B-C1B-NB	10.22	117.08	110.23
28	BQ	619	XAT	C15-C14-C13	-10.19	112.77	127.31
23	g	601	CHL	C2B-C1B-NB	10.19	117.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	7	318	XAT	C15-C14-C13	-10.18	112.78	127.31
23	e	601	CHL	C2B-C1B-NB	10.18	117.06	110.23
23	Au	609	CHL	C2B-C1B-NB	10.18	117.06	110.23
28	n	619	XAT	C15-C14-C13	-10.17	112.79	127.31
28	AB	312	XAT	C35-C34-C33	-10.16	112.81	127.31
23	6	606	CHL	C2B-C1B-NB	10.16	117.05	110.23
28	5	619	XAT	C31-C30-C29	-10.16	112.81	127.31
23	9	601	CHL	C2B-C1B-NB	10.14	117.03	110.23
28	8	312	XAT	C35-C34-C33	-10.13	112.86	127.31
23	BU	607	CHL	C2B-C1B-NB	10.11	117.01	110.23
23	BH	601	CHL	C2B-C1B-NB	10.10	117.01	110.23
23	5	601	CHL	C2B-C1B-NB	10.09	117.00	110.23
23	r	607	CHL	C2B-C1B-NB	10.09	117.00	110.23
28	BQ	619	XAT	C11-C10-C9	-10.08	112.92	127.31
28	y	301	XAT	C35-C34-C33	-10.07	112.93	127.31
28	g	619	XAT	C35-C34-C33	-10.07	112.94	127.31
28	BJ	619	XAT	C35-C34-C33	-10.06	112.95	127.31
28	7	318	XAT	C35-C34-C33	-10.06	112.95	127.31
23	Au	607	CHL	C2B-C1B-NB	10.05	116.97	110.23
23	9	606	CHL	C2B-C1B-NB	10.05	116.97	110.23
28	G	619	XAT	C15-C14-C13	-10.05	112.97	127.31
28	Au	619	XAT	C15-C14-C13	-10.05	112.97	127.31
28	r	616	XAT	C15-C14-C13	-10.05	112.97	127.31
28	AA	318	XAT	C35-C34-C33	-10.04	112.98	127.31
28	AB	312	XAT	C15-C14-C13	-10.04	112.98	127.31
28	Ba	301	XAT	C35-C34-C33	-10.04	112.98	127.31
23	Y	308	CHL	C2B-C1B-NB	10.03	116.96	110.23
28	y	301	XAT	C31-C30-C29	-10.01	113.02	127.31
28	Y	301	XAT	C15-C14-C13	-10.01	113.03	127.31
23	g	605	CHL	C2B-C1B-NB	10.00	116.94	110.23
28	BB	301	XAT	C15-C14-C13	-10.00	113.04	127.31
28	g	619	XAT	C15-C14-C13	-9.98	113.07	127.31
28	n	619	XAT	C11-C10-C9	-9.97	113.08	127.31
23	N	607	CHL	C2B-C1B-NB	9.96	116.91	110.23
23	BJ	605	CHL	C2B-C1B-NB	9.96	116.91	110.23
23	A2	609	CHL	C2B-C1B-NB	9.95	116.90	110.23
28	r	616	XAT	C11-C10-C9	-9.95	113.11	127.31
28	8	312	XAT	C15-C14-C13	-9.94	113.12	127.31
23	A2	607	CHL	C2B-C1B-NB	9.94	116.90	110.23
23	BJ	608	CHL	C2B-C1B-NB	9.94	116.89	110.23
28	Ba	301	XAT	C31-C30-C29	-9.93	113.14	127.31
28	BJ	619	XAT	C15-C14-C13	-9.93	113.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	308	CHL	C2B-C1B-NB	9.92	116.88	110.23
28	7	318	XAT	C11-C10-C9	-9.92	113.16	127.31
28	AA	318	XAT	C11-C10-C9	-9.91	113.16	127.31
28	BU	616	XAT	C11-C10-C9	-9.91	113.17	127.31
23	g	608	CHL	C2B-C1B-NB	9.91	116.88	110.23
23	Y	307	CHL	C2B-C1B-NB	9.91	116.87	110.23
23	BB	302	CHL	C2B-C1B-NB	9.90	116.87	110.23
28	BU	616	XAT	C15-C14-C13	-9.89	113.19	127.31
28	9	619	XAT	C11-C10-C9	-9.89	113.20	127.31
23	n	605	CHL	C2B-C1B-NB	9.88	116.85	110.23
23	BB	307	CHL	C2B-C1B-NB	9.87	116.85	110.23
23	BQ	605	CHL	C2B-C1B-NB	9.86	116.84	110.23
23	N	601	CHL	C2B-C1B-NB	9.86	116.84	110.23
23	A2	601	CHL	C2B-C1B-NB	9.85	116.83	110.23
28	n	619	XAT	C35-C34-C33	-9.83	113.28	127.31
23	A6	601	CHL	C2B-C1B-NB	9.82	116.81	110.23
28	AB	312	XAT	C31-C30-C29	-9.81	113.30	127.31
28	8	312	XAT	C31-C30-C29	-9.81	113.31	127.31
23	G	606	CHL	C2B-C1B-NB	9.81	116.81	110.23
23	N	609	CHL	C2B-C1B-NB	9.80	116.80	110.23
23	Y	302	CHL	C2B-C1B-NB	9.80	116.80	110.23
23	BV	606	CHL	C2B-C1B-NB	9.80	116.80	110.23
28	BU	616	XAT	C35-C34-C33	-9.79	113.33	127.31
23	S	605	CHL	C2B-C1B-NB	9.79	116.80	110.23
28	BQ	619	XAT	C35-C34-C33	-9.79	113.34	127.31
23	s	606	CHL	C2B-C1B-NB	9.77	116.78	110.23
23	A6	605	CHL	C2B-C1B-NB	9.77	116.78	110.23
28	A2	619	XAT	C11-C10-C9	-9.77	113.37	127.31
28	N	619	XAT	C35-C34-C33	-9.75	113.39	127.31
23	S	606	CHL	C2B-C1B-NB	9.75	116.77	110.23
28	A2	619	XAT	C35-C34-C33	-9.75	113.40	127.31
23	A6	606	CHL	C2B-C1B-NB	9.73	116.76	110.23
23	n	609	CHL	C2B-C1B-NB	9.72	116.75	110.23
28	r	616	XAT	C35-C34-C33	-9.71	113.45	127.31
28	N	619	XAT	C11-C10-C9	-9.71	113.45	127.31
23	S	601	CHL	C2B-C1B-NB	9.71	116.74	110.23
23	r	605	CHL	C2B-C1B-NB	9.70	116.73	110.23
23	Au	606	CHL	C2B-C1B-NB	9.69	116.73	110.23
28	BU	616	XAT	C31-C30-C29	-9.68	113.49	127.31
28	y	301	XAT	C11-C10-C9	-9.68	113.50	127.31
23	BB	310	CHL	C2B-C1B-NB	9.68	116.72	110.23
23	Y	309	CHL	C2B-C1B-NB	9.66	116.71	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	607	CHL	C2B-C1B-NB	9.65	116.70	110.23
23	BJ	606	CHL	C2B-C1B-NB	9.65	116.70	110.23
23	BU	605	CHL	C2B-C1B-NB	9.65	116.70	110.23
23	8	307	CHL	C2B-C1B-NB	9.64	116.70	110.23
28	Ba	301	XAT	C11-C10-C9	-9.63	113.57	127.31
23	6	607	CHL	C2B-C1B-NB	9.63	116.69	110.23
28	r	616	XAT	C31-C30-C29	-9.63	113.57	127.31
23	BQ	609	CHL	C2B-C1B-NB	9.62	116.68	110.23
23	AB	305	CHL	C2B-C1B-NB	9.62	116.68	110.23
23	r	606	CHL	C2B-C1B-NB	9.61	116.67	110.23
23	Au	605	CHL	C2B-C1B-NB	9.60	116.67	110.23
23	Y	310	CHL	C2B-C1B-NB	9.59	116.66	110.23
23	g	606	CHL	C2B-C1B-NB	9.56	116.64	110.23
23	BU	606	CHL	C2B-C1B-NB	9.56	116.64	110.23
23	0	607	CHL	C2B-C1B-NB	9.55	116.63	110.23
23	BB	309	CHL	C2B-C1B-NB	9.55	116.63	110.23
23	5	608	CHL	C2B-C1B-NB	9.53	116.62	110.23
23	8	305	CHL	C2B-C1B-NB	9.52	116.61	110.23
23	A2	606	CHL	C2B-C1B-NB	9.51	116.61	110.23
28	Y	301	XAT	C31-C30-C29	-9.51	113.74	127.31
28	Y	301	XAT	C35-C34-C33	-9.48	113.78	127.31
23	G	601	CHL	C2B-C1B-NB	9.46	116.58	110.23
28	BB	301	XAT	C35-C34-C33	-9.45	113.82	127.31
23	BV	601	CHL	C2B-C1B-NB	9.44	116.56	110.23
23	7	309	CHL	C2B-C1B-NB	9.44	116.56	110.23
23	5	607	CHL	C2B-C1B-NB	9.44	116.56	110.23
28	BB	301	XAT	C31-C30-C29	-9.44	113.84	127.31
23	G	605	CHL	C2B-C1B-NB	9.43	116.56	110.23
23	0	609	CHL	C2B-C1B-NB	9.43	116.56	110.23
28	n	619	XAT	C31-C30-C29	-9.43	113.85	127.31
23	n	601	CHL	C2B-C1B-NB	9.42	116.55	110.23
23	BQ	601	CHL	C2B-C1B-NB	9.42	116.55	110.23
23	9	608	CHL	C2B-C1B-NB	9.42	116.55	110.23
23	s	601	CHL	C2B-C1B-NB	9.42	116.55	110.23
23	AA	309	CHL	C2B-C1B-NB	9.40	116.53	110.23
28	7	301	XAT	C35-C34-C33	-9.39	113.90	127.31
23	Ba	302	CHL	C2B-C1B-NB	9.36	116.51	110.23
28	G	619	XAT	C11-C10-C9	-9.34	113.97	127.31
23	y	302	CHL	C2B-C1B-NB	9.34	116.49	110.23
23	0	608	CHL	C2B-C1B-NB	9.34	116.49	110.23
23	Au	601	CHL	C2B-C1B-NB	9.34	116.49	110.23
23	N	606	CHL	C2B-C1B-NB	9.33	116.49	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	AA	301	XAT	C35-C34-C33	-9.32	114.01	127.31
28	Au	619	XAT	C11-C10-C9	-9.32	114.01	127.31
23	S	607	CHL	C2B-C1B-NB	9.31	116.47	110.23
28	BQ	619	XAT	C31-C30-C29	-9.30	114.03	127.31
23	G	608	CHL	C2B-C1B-NB	9.29	116.46	110.23
23	BB	306	CHL	C2B-C1B-NB	9.28	116.45	110.23
23	Au	608	CHL	C2B-C1B-NB	9.26	116.44	110.23
23	AA	307	CHL	C2B-C1B-NB	9.25	116.43	110.23
23	Y	306	CHL	C2B-C1B-NB	9.24	116.43	110.23
23	6	605	CHL	C2B-C1B-NB	9.23	116.42	110.23
23	N	605	CHL	C2B-C1B-NB	9.22	116.41	110.23
23	r	613	CHL	C2B-C1B-NB	9.22	116.41	110.23
23	A2	608	CHL	C2B-C1B-NB	9.22	116.41	110.23
23	7	307	CHL	C2B-C1B-NB	9.21	116.41	110.23
23	6	608	CHL	C2B-C1B-NB	9.20	116.40	110.23
23	0	605	CHL	C2B-C1B-NB	9.18	116.39	110.23
28	5	619	XAT	C7-C8-C9	-9.18	111.29	125.53
23	5	605	CHL	C2B-C1B-NB	9.17	116.38	110.23
23	8	304	CHL	C2B-C1B-NB	9.17	116.38	110.23
23	AA	302	CHL	C2B-C1B-NB	9.16	116.37	110.23
23	AB	307	CHL	C2B-C1B-NB	9.16	116.37	110.23
23	n	608	CHL	C2B-C1B-NB	9.15	116.36	110.23
23	N	608	CHL	C2B-C1B-NB	9.15	116.36	110.23
23	BQ	608	CHL	C2B-C1B-NB	9.14	116.36	110.23
28	9	619	XAT	C7-C8-C9	-9.13	111.36	125.53
28	Y	301	XAT	C11-C10-C9	-9.13	114.27	127.31
23	9	605	CHL	C2B-C1B-NB	9.13	116.35	110.23
23	Ba	306	CHL	C2B-C1B-NB	9.12	116.34	110.23
28	BB	301	XAT	C11-C10-C9	-9.11	114.31	127.31
28	BJ	619	XAT	C11-C10-C9	-9.10	114.32	127.31
28	7	301	XAT	C11-C10-C9	-9.10	114.32	127.31
23	y	306	CHL	C2B-C1B-NB	9.10	116.33	110.23
28	AA	301	XAT	C11-C10-C9	-9.09	114.33	127.31
23	7	302	CHL	C2B-C1B-NB	9.09	116.33	110.23
28	g	619	XAT	C11-C10-C9	-9.09	114.34	127.31
28	7	301	XAT	C31-C30-C29	-9.08	114.35	127.31
23	BV	605	CHL	C2B-C1B-NB	9.08	116.32	110.23
28	AA	301	XAT	C31-C30-C29	-9.08	114.36	127.31
23	6	609	CHL	C2B-C1B-NB	9.08	116.32	110.23
23	A2	605	CHL	C2B-C1B-NB	9.07	116.31	110.23
28	g	619	XAT	C31-C30-C29	-9.07	114.36	127.31
23	AB	304	CHL	C2B-C1B-NB	9.06	116.30	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	619	XAT	C35-C34-C33	-9.05	114.39	127.31
28	BJ	619	XAT	C31-C30-C29	-9.05	114.39	127.31
23	BU	613	CHL	C2B-C1B-NB	9.05	116.30	110.23
23	s	605	CHL	C2B-C1B-NB	9.03	116.28	110.23
23	AB	307	CHL	CMD-C2D-C1D	9.01	140.60	124.71
23	6	601	CHL	C2B-C1B-NB	8.96	116.24	110.23
28	G	619	XAT	C31-C30-C29	-8.95	114.53	127.31
28	Au	619	XAT	C31-C30-C29	-8.91	114.60	127.31
23	5	606	CHL	CMD-C2D-C1D	8.90	140.40	124.71
23	A6	607	CHL	C2B-C1B-NB	8.90	116.20	110.23
28	Au	619	XAT	C35-C34-C33	-8.88	114.64	127.31
28	9	619	XAT	C15-C14-C13	-8.87	114.64	127.31
28	G	619	XAT	C35-C34-C33	-8.87	114.65	127.31
23	BV	607	CHL	C2B-C1B-NB	8.86	116.17	110.23
28	9	619	XAT	C38-C25-C26	-8.85	107.43	122.26
23	s	607	CHL	C2B-C1B-NB	8.85	116.16	110.23
28	5	619	XAT	C38-C25-C26	-8.83	107.47	122.26
23	Ba	307	CHL	C2B-C1B-NB	8.81	116.14	110.23
23	g	609	CHL	C2B-C1B-NB	8.81	116.14	110.23
23	0	601	CHL	C2B-C1B-NB	8.81	116.14	110.23
23	BJ	609	CHL	C2B-C1B-NB	8.79	116.12	110.23
23	AA	310	CHL	C2B-C1B-NB	8.78	116.12	110.23
23	9	606	CHL	CMD-C2D-C1D	8.78	140.19	124.71
23	S	607	CHL	C2C-C3C-C4C	-8.78	100.23	106.49
23	N	609	CHL	CMD-C2D-C1D	8.77	140.17	124.71
23	A2	609	CHL	CMD-C2D-C1D	8.77	140.17	124.71
23	0	609	CHL	CMD-C2D-C1D	8.76	140.14	124.71
23	7	310	CHL	C2B-C1B-NB	8.74	116.09	110.23
23	n	606	CHL	C2B-C1B-NB	8.73	116.08	110.23
28	N	619	XAT	C31-C30-C29	-8.69	114.91	127.31
23	A6	607	CHL	C2C-C3C-C4C	-8.67	100.31	106.49
28	A2	619	XAT	C31-C30-C29	-8.67	114.94	127.31
23	BU	613	CHL	CMD-C2D-C1D	8.67	139.99	124.71
23	y	307	CHL	C2B-C1B-NB	8.66	116.04	110.23
23	AB	306	CHL	C2B-C1B-NB	8.66	116.04	110.23
23	G	609	CHL	C2B-C1B-NB	8.65	116.03	110.23
23	6	609	CHL	CMD-C2D-C1D	8.64	139.94	124.71
23	5	609	CHL	C2B-C1B-NB	8.63	116.02	110.23
23	r	613	CHL	CMD-C2D-C1D	8.63	139.91	124.71
23	8	307	CHL	CMD-C2D-C1D	8.61	139.88	124.71
23	BJ	609	CHL	CMD-C2D-C1D	8.60	139.88	124.71
23	y	309	CHL	C2B-C1B-NB	8.58	115.98	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	g	609	CHL	CMD-C2D-C1D	8.58	139.83	124.71
23	n	609	CHL	CMD-C2D-C1D	8.57	139.81	124.71
23	8	306	CHL	C2B-C1B-NB	8.57	115.98	110.23
23	BQ	609	CHL	CMD-C2D-C1D	8.56	139.81	124.71
38	a	409	PHO	C4D-CHA-CBD	-8.56	104.64	108.52
23	0	609	CHL	C2C-C3C-C4C	-8.56	100.39	106.49
23	BQ	606	CHL	C2B-C1B-NB	8.56	115.97	110.23
23	Y	310	CHL	CMD-C2D-C1D	8.54	139.77	124.71
23	Ba	309	CHL	C2B-C1B-NB	8.54	115.96	110.23
23	7	306	CHL	C2B-C1B-NB	8.52	115.95	110.23
23	5	609	CHL	CMD-C2D-C1D	8.52	139.73	124.71
23	BU	605	CHL	CMD-C2D-C1D	8.49	139.68	124.71
23	r	606	CHL	CMD-C2D-C1D	8.49	139.67	124.71
23	AA	306	CHL	C2B-C1B-NB	8.49	115.92	110.23
23	5	609	CHL	C2C-C3C-C4C	-8.48	100.44	106.49
23	BU	606	CHL	CMD-C2D-C1D	8.48	139.66	124.71
23	s	605	CHL	CMD-C2D-C1D	8.47	139.64	124.71
23	r	605	CHL	CMD-C2D-C1D	8.46	139.62	124.71
23	9	601	CHL	CMD-C2D-C1D	8.46	139.62	124.71
23	5	601	CHL	CMD-C2D-C1D	8.44	139.59	124.71
23	9	609	CHL	C2C-C3C-C4C	-8.44	100.47	106.49
23	9	609	CHL	C2B-C1B-NB	8.43	115.89	110.23
23	7	309	CHL	CMD-C2D-C1D	8.43	139.57	124.71
38	BD	409	PHO	C4D-CHA-CBD	-8.43	104.70	108.52
23	AA	309	CHL	CMD-C2D-C1D	8.42	139.55	124.71
23	A2	601	CHL	CMD-C2D-C1D	8.41	139.53	124.71
23	6	608	CHL	CMD-C2D-C1D	8.41	139.53	124.71
23	A2	607	CHL	CMD-C2D-C1D	8.40	139.52	124.71
23	y	309	CHL	CMD-C2D-C1D	8.39	139.50	124.71
23	N	607	CHL	CMD-C2D-C1D	8.38	139.48	124.71
23	A2	606	CHL	CMD-C2D-C1D	8.38	139.48	124.71
23	G	601	CHL	CMD-C2D-C1D	8.37	139.47	124.71
23	n	606	CHL	CMD-C2D-C1D	8.36	139.45	124.71
23	N	601	CHL	CMD-C2D-C1D	8.36	139.44	124.71
23	Au	601	CHL	CMD-C2D-C1D	8.35	139.44	124.71
23	BQ	605	CHL	CMD-C2D-C1D	8.35	139.43	124.71
23	BV	605	CHL	CMD-C2D-C1D	8.34	139.42	124.71
23	BB	302	CHL	CMD-C2D-C1D	8.34	139.41	124.71
23	BQ	606	CHL	CMD-C2D-C1D	8.34	139.41	124.71
23	9	605	CHL	CMD-C2D-C1D	8.34	139.41	124.71
23	9	609	CHL	CMD-C2D-C1D	8.34	139.40	124.71
23	BB	310	CHL	CMD-C2D-C1D	8.34	139.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	608	CHL	CMD-C2D-C1D	8.33	139.40	124.71
23	BB	306	CHL	CMD-C2D-C1D	8.33	139.39	124.71
23	G	608	CHL	CMD-C2D-C1D	8.33	139.39	124.71
23	n	605	CHL	CMD-C2D-C1D	8.32	139.38	124.71
23	N	606	CHL	CMD-C2D-C1D	8.32	139.38	124.71
23	5	608	CHL	CMD-C2D-C1D	8.32	139.37	124.71
23	S	607	CHL	CMD-C2D-C1D	8.31	139.37	124.71
23	N	608	CHL	CMD-C2D-C1D	8.31	139.36	124.71
23	0	605	CHL	CMD-C2D-C1D	8.31	139.35	124.71
23	AA	302	CHL	CMD-C2D-C1D	8.30	139.35	124.71
28	BU	616	XAT	C39-C29-C30	-8.30	111.30	122.92
23	Ba	306	CHL	CMD-C2D-C1D	8.30	139.34	124.71
23	G	606	CHL	CMD-C2D-C1D	8.29	139.33	124.71
23	BJ	605	CHL	CMD-C2D-C1D	8.29	139.33	124.71
23	6	605	CHL	CMD-C2D-C1D	8.29	139.33	124.71
23	Y	307	CHL	CMD-C2D-C1D	8.29	139.33	124.71
23	5	605	CHL	CMD-C2D-C1D	8.29	139.32	124.71
23	Au	609	CHL	CMD-C2D-C1D	8.29	139.32	124.71
23	Au	607	CHL	CMD-C2D-C1D	8.29	139.32	124.71
23	BB	307	CHL	CMD-C2D-C1D	8.29	139.32	124.71
23	0	608	CHL	CMD-C2D-C1D	8.28	139.31	124.71
23	Ba	309	CHL	CMD-C2D-C1D	8.28	139.31	124.71
23	Au	608	CHL	CMD-C2D-C1D	8.28	139.31	124.71
23	7	302	CHL	CMD-C2D-C1D	8.28	139.30	124.71
23	AB	304	CHL	CMD-C2D-C1D	8.28	139.30	124.71
23	BB	308	CHL	CMD-C2D-C1D	8.28	139.30	124.71
23	A2	608	CHL	CMD-C2D-C1D	8.27	139.28	124.71
23	N	605	CHL	CMD-C2D-C1D	8.26	139.28	124.71
23	g	605	CHL	CMD-C2D-C1D	8.26	139.28	124.71
23	BQ	607	CHL	CMD-C2D-C1D	8.26	139.28	124.71
23	Y	307	CHL	C2C-C3C-C4C	-8.26	100.60	106.49
23	Au	606	CHL	CMD-C2D-C1D	8.26	139.27	124.71
23	8	304	CHL	CMD-C2D-C1D	8.26	139.27	124.71
23	Y	306	CHL	CMD-C2D-C1D	8.26	139.27	124.71
23	A6	607	CHL	CMD-C2D-C1D	8.26	139.27	124.71
23	7	306	CHL	CMD-C2D-C1D	8.25	139.26	124.71
23	g	601	CHL	CMD-C2D-C1D	8.25	139.26	124.71
23	y	306	CHL	CMD-C2D-C1D	8.25	139.25	124.71
23	BJ	607	CHL	CMD-C2D-C1D	8.25	139.25	124.71
23	Y	302	CHL	CMD-C2D-C1D	8.25	139.25	124.71
23	Y	309	CHL	CMD-C2D-C1D	8.25	139.25	124.71
23	Ba	302	CHL	CMD-C2D-C1D	8.25	139.25	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	607	CHL	CMD-C2D-C1D	8.24	139.24	124.71
23	BJ	606	CHL	CMD-C2D-C1D	8.24	139.24	124.71
23	AA	308	CHL	CMD-C2D-C1D	8.24	139.23	124.71
23	BJ	601	CHL	CMD-C2D-C1D	8.24	139.23	124.71
23	g	607	CHL	CMD-C2D-C1D	8.24	139.23	124.71
23	G	607	CHL	CMD-C2D-C1D	8.24	139.23	124.71
23	A6	606	CHL	CMD-C2D-C1D	8.24	139.23	124.71
23	S	606	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	g	606	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	7	308	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	y	302	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	A2	605	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	AA	306	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	BU	607	CHL	CMD-C2D-C1D	8.23	139.21	124.71
23	Y	308	CHL	CMD-C2D-C1D	8.22	139.20	124.71
28	AB	312	XAT	C11-C10-C9	-8.22	115.58	127.31
23	7	310	CHL	CMD-C2D-C1D	8.22	139.19	124.71
28	AA	301	XAT	C27-C28-C29	-8.21	112.79	125.53
23	S	605	CHL	CMD-C2D-C1D	8.21	139.18	124.71
23	y	308	CHL	CMD-C2D-C1D	8.21	139.17	124.71
23	BB	307	CHL	C2C-C3C-C4C	-8.20	100.64	106.49
23	A6	605	CHL	CMD-C2D-C1D	8.20	139.16	124.71
23	BJ	608	CHL	CMD-C2D-C1D	8.19	139.15	124.71
23	AA	310	CHL	CMD-C2D-C1D	8.19	139.15	124.71
23	n	608	CHL	CMD-C2D-C1D	8.19	139.14	124.71
23	g	608	CHL	CMD-C2D-C1D	8.19	139.14	124.71
23	BQ	608	CHL	CMD-C2D-C1D	8.18	139.13	124.71
23	BB	309	CHL	CMD-C2D-C1D	8.17	139.11	124.71
28	8	312	XAT	C11-C10-C9	-8.17	115.66	127.31
23	y	310	CHL	C2B-C1B-NB	8.17	115.71	110.23
23	Ba	308	CHL	CMD-C2D-C1D	8.17	139.10	124.71
23	y	310	CHL	CMD-C2D-C1D	8.16	139.09	124.71
23	r	607	CHL	CMD-C2D-C1D	8.15	139.08	124.71
28	r	616	XAT	C39-C29-C30	-8.13	111.53	122.92
23	Au	605	CHL	CMD-C2D-C1D	8.13	139.04	124.71
23	y	307	CHL	CMD-C2D-C1D	8.13	139.04	124.71
23	6	607	CHL	CMD-C2D-C1D	8.13	139.03	124.71
23	Ba	307	CHL	CMD-C2D-C1D	8.12	139.02	124.71
23	G	605	CHL	CMD-C2D-C1D	8.11	139.01	124.71
23	BU	607	CHL	C2C-C3C-C4C	-8.11	100.71	106.49
23	AA	307	CHL	CMD-C2D-C1D	8.11	139.01	124.71
23	AA	302	CHL	C2C-C3C-C4C	-8.10	100.72	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A6	605	CHL	C2C-C3C-C4C	-8.10	100.72	106.49
23	7	307	CHL	CMD-C2D-C1D	8.09	138.96	124.71
23	8	305	CHL	CMD-C2D-C1D	8.07	138.94	124.71
23	9	601	CHL	C2C-C3C-C4C	-8.05	100.75	106.49
23	BQ	601	CHL	CMD-C2D-C1D	8.05	138.90	124.71
28	7	301	XAT	C27-C28-C29	-8.05	113.04	125.53
23	AB	305	CHL	CMD-C2D-C1D	8.05	138.90	124.71
23	S	605	CHL	C2C-C3C-C4C	-8.04	100.76	106.49
23	n	601	CHL	CMD-C2D-C1D	8.04	138.88	124.71
23	G	609	CHL	CMD-C2D-C1D	8.03	138.86	124.71
28	AA	318	XAT	C7-C8-C9	-8.02	113.08	125.53
23	0	607	CHL	CMD-C2D-C1D	8.02	138.84	124.71
23	Ba	310	CHL	C2B-C1B-NB	8.01	115.60	110.23
23	6	606	CHL	CMD-C2D-C1D	8.01	138.83	124.71
28	AA	318	XAT	C27-C28-C29	-8.01	113.10	125.53
28	7	318	XAT	C7-C8-C9	-8.00	113.12	125.53
23	0	606	CHL	CMD-C2D-C1D	7.99	138.79	124.71
23	r	607	CHL	C2C-C3C-C4C	-7.98	100.80	106.49
23	BV	607	CHL	CMD-C2D-C1D	7.97	138.76	124.71
23	0	601	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
28	7	318	XAT	C27-C28-C29	-7.96	113.17	125.53
28	r	616	XAT	C7-C8-C9	-7.96	113.18	125.53
23	s	607	CHL	CMD-C2D-C1D	7.96	138.74	124.71
23	5	601	CHL	C2C-C3C-C4C	-7.96	100.82	106.49
23	BB	309	CHL	C2C-C3C-C4C	-7.95	100.82	106.49
23	7	302	CHL	C2C-C3C-C4C	-7.95	100.82	106.49
23	Ba	310	CHL	CMD-C2D-C1D	7.95	138.72	124.71
23	BH	601	CHL	CMD-C2D-C1D	7.94	138.71	124.71
28	BU	616	XAT	C7-C8-C9	-7.94	113.21	125.53
23	6	601	CHL	CMD-C2D-C1D	7.93	138.69	124.71
23	0	606	CHL	C2C-C3C-C4C	-7.93	100.83	106.49
23	8	306	CHL	CMD-C2D-C1D	7.92	138.67	124.71
23	0	601	CHL	CMD-C2D-C1D	7.92	138.67	124.71
23	Ba	307	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
23	e	601	CHL	CMD-C2D-C1D	7.90	138.64	124.71
23	7	307	CHL	C2C-C3C-C4C	-7.88	100.87	106.49
23	6	606	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
23	A2	607	CHL	C2C-C3C-C4C	-7.86	100.89	106.49
23	y	307	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
28	A2	619	XAT	C7-C8-C9	-7.84	113.37	125.53
23	AA	307	CHL	C2C-C3C-C4C	-7.83	100.91	106.49
23	g	606	CHL	C2C-C3C-C4C	-7.83	100.91	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	601	CHL	C2C-C3C-C4C	-7.82	100.91	106.49
23	AB	306	CHL	CMD-C2D-C1D	7.82	138.49	124.71
23	BV	606	CHL	CMD-C2D-C1D	7.82	138.49	124.71
23	Au	606	CHL	C2C-C3C-C4C	-7.81	100.92	106.49
23	Au	607	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
23	G	606	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
28	BB	301	XAT	C7-C8-C9	-7.79	113.44	125.53
23	6	609	CHL	C2C-C3C-C4C	-7.79	100.94	106.49
23	Y	309	CHL	C2C-C3C-C4C	-7.79	100.94	106.49
28	AB	312	XAT	C20-C13-C14	-7.77	112.04	122.92
28	N	619	XAT	C7-C8-C9	-7.76	113.48	125.53
23	s	606	CHL	CMD-C2D-C1D	7.76	138.39	124.71
28	Y	301	XAT	C7-C8-C9	-7.76	113.50	125.53
23	N	607	CHL	C2C-C3C-C4C	-7.75	100.96	106.49
23	BJ	606	CHL	C2C-C3C-C4C	-7.75	100.97	106.49
23	A6	607	CHL	CAC-C3C-C4C	7.74	134.85	124.81
28	8	312	XAT	C20-C13-C14	-7.74	112.08	122.92
23	N	605	CHL	C2C-C3C-C4C	-7.73	100.98	106.49
23	A2	605	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
23	0	607	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
28	9	619	XAT	C26-C27-C28	-7.70	109.70	125.99
23	7	309	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
38	A	409	PHO	C4D-CHA-CBD	-7.70	105.04	108.52
28	5	619	XAT	C26-C27-C28	-7.69	109.74	125.99
23	G	607	CHL	C2C-C3C-C4C	-7.67	101.02	106.49
23	Au	605	CHL	C2C-C3C-C4C	-7.67	101.02	106.49
23	5	607	CHL	CMD-C2D-C1D	7.66	138.22	124.71
23	S	601	CHL	CMD-C2D-C1D	7.66	138.21	124.71
23	BV	601	CHL	CMD-C2D-C1D	7.65	138.20	124.71
28	n	619	XAT	C7-C8-C9	-7.65	113.66	125.53
23	s	601	CHL	CMD-C2D-C1D	7.64	138.18	124.71
23	9	607	CHL	C2C-C3C-C4C	-7.64	101.04	106.49
23	A2	606	CHL	C2C-C3C-C4C	-7.64	101.04	106.49
23	BJ	608	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
28	8	312	XAT	C19-C9-C10	-7.63	112.24	122.92
23	A6	601	CHL	CMD-C2D-C1D	7.62	138.15	124.71
23	5	606	CHL	C2C-C3C-C4C	-7.62	101.05	106.49
23	AA	309	CHL	C2C-C3C-C4C	-7.62	101.05	106.49
23	g	609	CHL	CHD-C1D-ND	-7.62	117.45	124.45
28	BQ	619	XAT	C7-C8-C9	-7.62	113.71	125.53
23	A6	607	CHL	CHD-C1D-ND	-7.61	117.46	124.45
24	6	604	CLA	C4A-NA-C1A	7.61	110.13	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	AB	312	XAT	C19-C9-C10	-7.60	112.27	122.92
38	R	408	PHO	C4D-CHA-CBD	-7.58	105.09	108.52
23	9	607	CHL	CMD-C2D-C1D	7.58	138.06	124.71
23	BJ	609	CHL	CHD-C1D-ND	-7.57	117.50	124.45
23	9	606	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
23	g	608	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
28	Y	301	XAT	C27-C28-C29	-7.55	113.82	125.53
28	BB	301	XAT	C27-C28-C29	-7.55	113.82	125.53
23	0	608	CHL	C2C-C3C-C4C	-7.54	101.11	106.49
28	Ba	301	XAT	C7-C8-C9	-7.54	113.83	125.53
23	Ba	308	CHL	C2C-C3C-C4C	-7.54	101.11	106.49
23	BV	607	CHL	C2C-C3C-C4C	-7.54	101.12	106.49
23	s	601	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
23	g	605	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
23	BJ	605	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
23	S	601	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
23	BQ	608	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
23	BQ	607	CHL	C2C-C3C-C4C	-7.52	101.12	106.49
28	Ba	301	XAT	C27-C28-C29	-7.52	113.86	125.53
23	BV	601	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
28	y	301	XAT	C27-C28-C29	-7.52	113.86	125.53
23	N	606	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
23	s	606	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
23	n	607	CHL	C2C-C3C-C4C	-7.51	101.13	106.49
28	BB	301	XAT	C39-C29-C30	-7.51	112.40	122.92
23	s	607	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
28	r	616	XAT	C27-C28-C29	-7.51	113.88	125.53
23	n	606	CHL	C2C-C3C-C4C	-7.50	101.14	106.49
23	A2	608	CHL	C2C-C3C-C4C	-7.50	101.14	106.49
23	BB	308	CHL	C2C-C3C-C4C	-7.50	101.14	106.49
28	5	619	XAT	C19-C9-C10	-7.49	112.43	122.92
23	Y	308	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
24	7	303	CLA	C4A-NA-C1A	7.48	110.07	106.71
28	BU	616	XAT	C27-C28-C29	-7.48	113.92	125.53
23	N	608	CHL	C2C-C3C-C4C	-7.48	101.15	106.49
23	n	608	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
23	BU	613	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
28	BU	616	XAT	C20-C13-C14	-7.48	112.44	122.92
23	BV	606	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
23	BQ	605	CHL	C2C-C3C-C4C	-7.47	101.16	106.49
24	BE	609	CLA	C4A-NA-C1A	7.47	110.06	106.71
24	B	611	CLA	C4A-NA-C1A	7.47	110.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C4A-NA-C1A	7.47	110.06	106.71
23	BH	601	CHL	C2C-C3C-C4C	-7.47	101.17	106.49
28	Y	301	XAT	C39-C29-C30	-7.46	112.47	122.92
23	BJ	607	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
28	AB	312	XAT	C27-C28-C29	-7.45	113.97	125.53
23	n	605	CHL	C2C-C3C-C4C	-7.45	101.18	106.49
28	n	619	XAT	C27-C28-C29	-7.45	113.97	125.53
23	BQ	606	CHL	C2C-C3C-C4C	-7.44	101.18	106.49
28	BJ	619	XAT	C7-C8-C9	-7.44	113.98	125.53
28	g	619	XAT	C7-C8-C9	-7.44	113.99	125.53
28	y	301	XAT	C7-C8-C9	-7.44	113.99	125.53
23	AB	307	CHL	CHD-C1D-ND	-7.44	117.62	124.45
28	BU	616	XAT	C18-C5-C6	-7.44	109.80	122.26
23	g	607	CHL	C2C-C3C-C4C	-7.43	101.19	106.49
24	6	612	CLA	C4A-NA-C1A	7.42	110.04	106.71
28	A2	619	XAT	C27-C28-C29	-7.42	114.02	125.53
28	r	616	XAT	C20-C13-C14	-7.42	112.53	122.92
28	5	619	XAT	C27-C28-C29	-7.41	114.03	125.53
23	S	606	CHL	C2C-C3C-C4C	-7.41	101.20	106.49
28	8	312	XAT	C27-C28-C29	-7.41	114.03	125.53
23	A6	606	CHL	C2C-C3C-C4C	-7.41	101.21	106.49
24	AA	303	CLA	C4A-NA-C1A	7.40	110.03	106.71
23	Ba	306	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
23	G	605	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
23	9	608	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
24	b	609	CLA	C4A-NA-C1A	7.40	110.03	106.71
24	r	604	CLA	C4A-NA-C1A	7.40	110.03	106.71
28	BU	616	XAT	C19-C9-C10	-7.39	112.57	122.92
28	r	616	XAT	C19-C9-C10	-7.39	112.57	122.92
23	y	306	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
23	AB	307	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
28	9	619	XAT	C19-C9-C10	-7.39	112.58	122.92
23	BJ	601	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
23	y	308	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
23	BV	605	CHL	C2C-C3C-C4C	-7.37	101.23	106.49
23	AA	302	CHL	CHD-C1D-ND	-7.37	117.68	124.45
28	9	619	XAT	C27-C28-C29	-7.37	114.09	125.53
24	v	611	CLA	C4A-NA-C1A	7.37	110.02	106.71
28	BQ	619	XAT	C19-C9-C10	-7.37	112.60	122.92
23	AB	304	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
28	BQ	619	XAT	C27-C28-C29	-7.36	114.10	125.53
23	e	601	CHL	C2C-C3C-C4C	-7.36	101.24	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	y	310	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
23	Au	609	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
23	5	608	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
23	AA	308	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
23	Ba	302	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
28	N	619	XAT	C27-C28-C29	-7.34	114.14	125.53
23	9	605	CHL	C2C-C3C-C4C	-7.34	101.25	106.49
23	A6	601	CHL	C2C-C3C-C4C	-7.34	101.25	106.49
28	Au	619	XAT	C27-C28-C29	-7.34	114.14	125.53
28	G	619	XAT	C7-C8-C9	-7.34	114.14	125.53
28	8	312	XAT	C18-C5-C6	-7.34	109.96	122.26
28	r	616	XAT	C18-C5-C6	-7.34	109.96	122.26
24	A6	612	CLA	C4A-NA-C1A	7.34	110.00	106.71
24	BF	506	CLA	C4A-NA-C1A	7.34	110.00	106.71
24	c	503	CLA	C4A-NA-C1A	7.33	110.00	106.71
28	AA	301	XAT	C7-C8-C9	-7.33	114.16	125.53
28	G	619	XAT	C27-C28-C29	-7.33	114.16	125.53
23	y	302	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
23	g	601	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
28	7	301	XAT	C7-C8-C9	-7.32	114.17	125.53
28	Au	619	XAT	C7-C8-C9	-7.32	114.17	125.53
24	BU	604	CLA	C4A-NA-C1A	7.30	109.99	106.71
23	5	605	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
23	6	608	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
23	AA	310	CHL	CHD-C1D-ND	-7.30	117.74	124.45
23	s	605	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
28	AB	312	XAT	C18-C5-C6	-7.30	110.03	122.26
23	BB	310	CHL	C2C-C3C-C4C	-7.30	101.29	106.49
24	BU	609	CLA	C4A-NA-C1A	7.30	109.99	106.71
28	AA	301	XAT	C20-C13-C14	-7.29	112.71	122.92
24	C	513	CLA	C4A-NA-C1A	7.29	109.98	106.71
23	7	308	CHL	C2C-C3C-C4C	-7.29	101.30	106.49
23	y	309	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
23	r	613	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
28	n	619	XAT	C19-C9-C10	-7.28	112.72	122.92
23	N	601	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
24	n	611	CLA	C4A-NA-C1A	7.27	109.98	106.71
24	0	612	CLA	C4A-NA-C1A	7.27	109.98	106.71
23	6	607	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
23	8	304	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
23	Y	310	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
24	1	513	CLA	C4A-NA-C1A	7.27	109.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	8	307	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
28	AB	312	XAT	C6-C7-C8	-7.27	110.63	125.99
23	G	601	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
28	7	301	XAT	C20-C13-C14	-7.25	112.76	122.92
24	b	610	CLA	C4A-NA-C1A	7.24	109.96	106.71
28	8	312	XAT	C6-C7-C8	-7.24	110.68	125.99
23	y	310	CHL	CHD-C1D-ND	-7.24	117.80	124.45
23	9	609	CHL	CHB-C1B-NB	-7.23	116.60	124.26
23	AB	306	CHL	C2C-C3C-C4C	-7.23	101.33	106.49
23	7	310	CHL	CHD-C1D-ND	-7.23	117.81	124.45
24	BF	503	CLA	C4A-NA-C1A	7.23	109.96	106.71
23	5	607	CHL	C2C-C3C-C4C	-7.23	101.34	106.49
23	7	302	CHL	CHD-C1D-ND	-7.22	117.82	124.45
24	B	614	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	8	303	CLA	C4A-NA-C1A	7.21	109.95	106.71
24	N	604	CLA	C4A-NA-C1A	7.21	109.95	106.71
23	Y	306	CHL	C2C-C3C-C4C	-7.20	101.35	106.49
23	Ba	309	CHL	C2C-C3C-C4C	-7.20	101.35	106.49
24	r	601	CLA	C4A-NA-C1A	7.20	109.94	106.71
23	8	306	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
23	Au	608	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
23	BQ	601	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
23	A2	601	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
23	6	605	CHL	C2C-C3C-C4C	-7.19	101.37	106.49
23	8	305	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
23	n	601	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
24	BD	410	CLA	C4A-NA-C1A	7.17	109.93	106.71
28	AB	312	XAT	C26-C27-C28	-7.17	110.83	125.99
23	6	609	CHL	CHB-C1B-NB	-7.17	116.67	124.26
24	BQ	611	CLA	C4A-NA-C1A	7.17	109.93	106.71
28	8	312	XAT	C26-C27-C28	-7.16	110.84	125.99
23	6	609	CHL	CHD-C1D-ND	-7.16	117.87	124.45
24	9	614	CLA	C4A-NA-C1A	7.16	109.92	106.71
24	AB	303	CLA	C4A-NA-C1A	7.15	109.92	106.71
23	A2	609	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
28	BU	616	XAT	C40-C33-C34	-7.15	112.91	122.92
24	A2	604	CLA	C4A-NA-C1A	7.14	109.92	106.71
23	r	606	CHL	C2C-C3C-C4C	-7.13	101.40	106.49
24	BF	509	CLA	C4A-NA-C1A	7.13	109.91	106.71
24	BF	514	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	G	608	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
24	S	612	CLA	C4A-NA-C1A	7.13	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	409	CLA	C4A-NA-C1A	7.12	109.91	106.71
24	c	506	CLA	C4A-NA-C1A	7.12	109.91	106.71
23	7	306	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
23	N	609	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
24	y	305	CLA	C4A-NA-C1A	7.10	109.90	106.71
24	v	614	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	BU	606	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
23	Au	601	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
23	Ba	310	CHL	CHD-C1D-ND	-7.10	117.93	124.45
24	a	410	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	0	605	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
24	6	611	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	Ba	310	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
23	AB	305	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
24	v	609	CLA	C4A-NA-C1A	7.07	109.89	106.71
23	BB	302	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
24	b	611	CLA	C4A-NA-C1A	7.07	109.88	106.71
23	AA	306	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
23	BB	306	CHL	C2C-C3C-C4C	-7.06	101.46	106.49
24	a	407	CLA	C4A-NA-C1A	7.06	109.88	106.71
24	BB	303	CLA	C4A-NA-C1A	7.05	109.88	106.71
24	A2	612	CLA	C4A-NA-C1A	7.05	109.88	106.71
24	BE	614	CLA	C4A-NA-C1A	7.05	109.88	106.71
24	BU	601	CLA	C4A-NA-C1A	7.05	109.88	106.71
28	AA	318	XAT	C40-C33-C34	-7.04	113.06	122.92
24	5	614	CLA	C4A-NA-C1A	7.04	109.87	106.71
24	r	602	CLA	C4A-NA-C1A	7.04	109.87	106.71
24	1	503	CLA	C4A-NA-C1A	7.04	109.87	106.71
28	BJ	619	XAT	C27-C28-C29	-7.03	114.62	125.53
24	G	603	CLA	C4A-NA-C1A	7.03	109.87	106.71
24	c	509	CLA	C4A-NA-C1A	7.03	109.87	106.71
24	BQ	612	CLA	C4A-NA-C1A	7.03	109.87	106.71
23	BJ	609	CHL	C2C-C3C-C4C	-7.03	101.48	106.49
24	B	602	CLA	C4A-NA-C1A	7.02	109.86	106.71
28	g	619	XAT	C27-C28-C29	-7.02	114.64	125.53
23	Y	302	CHL	C2C-C3C-C4C	-7.02	101.49	106.49
23	G	609	CHL	C2C-C3C-C4C	-7.02	101.49	106.49
24	N	613	CLA	C4A-NA-C1A	7.01	109.86	106.71
28	AA	318	XAT	C39-C29-C30	-7.01	113.10	122.92
24	n	612	CLA	C4A-NA-C1A	7.01	109.86	106.71
24	1	508	CLA	C4A-NA-C1A	7.01	109.86	106.71
23	G	609	CHL	CHD-C1D-ND	-7.01	118.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	g	609	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
24	A6	602	CLA	C4A-NA-C1A	7.00	109.85	106.71
28	A2	619	XAT	C19-C9-C10	-7.00	113.12	122.92
28	r	616	XAT	C40-C33-C34	-7.00	113.12	122.92
24	C	508	CLA	C4A-NA-C1A	7.00	109.85	106.71
24	b	605	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	A2	613	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	BJ	614	CLA	C4A-NA-C1A	6.99	109.85	106.71
28	5	619	XAT	C39-C29-C30	-6.99	113.13	122.92
24	A2	603	CLA	C4A-NA-C1A	6.99	109.85	106.71
28	7	318	XAT	C39-C29-C30	-6.98	113.14	122.92
24	r	609	CLA	C4A-NA-C1A	6.98	109.85	106.71
28	N	619	XAT	C19-C9-C10	-6.98	113.14	122.92
28	7	301	XAT	C40-C33-C34	-6.98	113.15	122.92
24	N	610	CLA	C4A-NA-C1A	6.98	109.84	106.71
24	N	612	CLA	C4A-NA-C1A	6.98	109.84	106.71
24	2	403	CLA	C4A-NA-C1A	6.98	109.84	106.71
23	0	609	CHL	CHB-C1B-NB	-6.97	116.88	124.26
28	BU	616	XAT	C6-C7-C8	-6.97	111.25	125.99
28	AA	301	XAT	C40-C33-C34	-6.97	113.16	122.92
23	r	613	CHL	CHD-C1D-ND	-6.97	118.05	124.45
24	b	614	CLA	C4A-NA-C1A	6.96	109.84	106.71
24	S	604	CLA	C4A-NA-C1A	6.96	109.83	106.71
24	0	611	CLA	C4A-NA-C1A	6.96	109.83	106.71
24	BE	605	CLA	C4A-NA-C1A	6.96	109.83	106.71
23	BU	613	CHL	CHD-C1D-ND	-6.96	118.06	124.45
24	I	102	CLA	C4A-NA-C1A	6.96	109.83	106.71
24	BF	511	CLA	C4A-NA-C1A	6.96	109.83	106.71
28	r	616	XAT	C6-C7-C8	-6.96	111.29	125.99
28	n	619	XAT	C26-C27-C28	-6.95	111.29	125.99
24	b	617	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	7	312	CLA	C4A-NA-C1A	6.95	109.83	106.71
28	9	619	XAT	C39-C29-C30	-6.95	113.19	122.92
24	BE	610	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	BF	507	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	B	613	CLA	C4A-NA-C1A	6.94	109.83	106.71
24	v	607	CLA	C4A-NA-C1A	6.94	109.83	106.71
28	Au	619	XAT	C40-C33-C34	-6.94	113.20	122.92
24	B	607	CLA	C4A-NA-C1A	6.94	109.83	106.71
24	Y	303	CLA	C4A-NA-C1A	6.93	109.82	106.71
24	r	614	CLA	C4A-NA-C1A	6.93	109.82	106.71
24	Ba	305	CLA	C4A-NA-C1A	6.93	109.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	313	CLA	C4A-NA-C1A	6.93	109.82	106.71
24	g	614	CLA	C4A-NA-C1A	6.93	109.82	106.71
28	7	318	XAT	C40-C33-C34	-6.93	113.22	122.92
24	BU	602	CLA	C4A-NA-C1A	6.93	109.82	106.71
24	N	603	CLA	C4A-NA-C1A	6.92	109.82	106.71
28	AA	301	XAT	C39-C29-C30	-6.92	113.22	122.92
24	s	611	CLA	C4A-NA-C1A	6.92	109.82	106.71
24	A6	603	CLA	C4A-NA-C1A	6.92	109.82	106.71
28	BQ	619	XAT	C26-C27-C28	-6.92	111.37	125.99
28	AA	318	XAT	C38-C25-C26	-6.91	110.67	122.26
28	n	619	XAT	C40-C33-C34	-6.91	113.24	122.92
24	B	604	CLA	C4A-NA-C1A	6.91	109.81	106.71
24	Au	610	CLA	C4A-NA-C1A	6.91	109.81	106.71
28	G	619	XAT	C40-C33-C34	-6.91	113.25	122.92
24	c	511	CLA	C4A-NA-C1A	6.90	109.81	106.71
28	BQ	619	XAT	C40-C33-C34	-6.90	113.25	122.92
24	Y	311	CLA	C4A-NA-C1A	6.90	109.81	106.71
24	v	604	CLA	C4A-NA-C1A	6.90	109.81	106.71
24	v	613	CLA	C4A-NA-C1A	6.90	109.81	106.71
24	BD	406	CLA	C4A-NA-C1A	6.90	109.81	106.71
28	7	318	XAT	C20-C13-C14	-6.90	113.26	122.92
24	BD	407	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	BV	606	CHL	O2D-CGD-CBD	6.89	123.52	111.27
24	BB	304	CLA	C4A-NA-C1A	6.89	109.81	106.71
24	Au	614	CLA	C4A-NA-C1A	6.89	109.80	106.71
24	A6	604	CLA	C4A-NA-C1A	6.89	109.80	106.71
28	AB	312	XAT	C40-C33-C34	-6.89	113.28	122.92
24	BF	513	CLA	C4A-NA-C1A	6.88	109.80	106.71
28	BB	301	XAT	C19-C9-C10	-6.88	113.28	122.92
23	s	606	CHL	O2D-CGD-CBD	6.88	123.49	111.27
24	c	507	CLA	C4A-NA-C1A	6.88	109.80	106.71
24	Aw	102	CLA	C4A-NA-C1A	6.88	109.80	106.71
24	Y	315	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	D	402	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	BE	617	CLA	C4A-NA-C1A	6.87	109.80	106.71
28	AA	318	XAT	C20-C13-C14	-6.87	113.30	122.92
24	BF	512	CLA	C4A-NA-C1A	6.87	109.79	106.71
24	G	602	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	A2	602	CLA	C4A-NA-C1A	6.86	109.79	106.71
28	A2	619	XAT	C39-C29-C30	-6.86	113.31	122.92
24	A	410	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	N	611	CLA	C4A-NA-C1A	6.85	109.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	312	CLA	C4A-NA-C1A	6.85	109.79	106.71
24	BB	315	CLA	C4A-NA-C1A	6.85	109.79	106.71
28	A2	619	XAT	C20-C13-C14	-6.85	113.33	122.92
28	AA	318	XAT	C26-C27-C28	-6.85	111.51	125.99
24	S	603	CLA	C4A-NA-C1A	6.85	109.78	106.71
24	C	503	CLA	C4A-NA-C1A	6.84	109.78	106.71
24	BF	508	CLA	C4A-NA-C1A	6.84	109.78	106.71
28	y	301	XAT	C6-C7-C8	-6.84	111.53	125.99
28	y	301	XAT	C39-C29-C30	-6.84	113.34	122.92
24	C	507	CLA	C4A-NA-C1A	6.84	109.78	106.71
28	8	312	XAT	C40-C33-C34	-6.84	113.34	122.92
24	BB	311	CLA	C4A-NA-C1A	6.84	109.78	106.71
28	AB	312	XAT	C39-C29-C30	-6.83	113.35	122.92
28	7	318	XAT	C26-C27-C28	-6.83	111.54	125.99
28	Y	301	XAT	C19-C9-C10	-6.83	113.35	122.92
24	Y	304	CLA	C4A-NA-C1A	6.83	109.78	106.71
28	7	301	XAT	C39-C29-C30	-6.83	113.35	122.92
24	1	507	CLA	C4A-NA-C1A	6.83	109.78	106.71
28	A2	619	XAT	C40-C33-C34	-6.83	113.36	122.92
28	8	312	XAT	C7-C8-C9	-6.83	114.93	125.53
28	AB	312	XAT	C7-C8-C9	-6.83	114.93	125.53
24	S	602	CLA	C4A-NA-C1A	6.83	109.78	106.71
24	Ba	313	CLA	C4A-NA-C1A	6.83	109.78	106.71
24	0	613	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	g	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
28	Y	301	XAT	C40-C33-C34	-6.82	113.37	122.92
24	v	602	CLA	C4A-NA-C1A	6.82	109.77	106.71
28	7	318	XAT	C38-C25-C26	-6.82	110.83	122.26
24	r	608	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	9	612	CLA	C4A-NA-C1A	6.82	109.77	106.71
28	n	619	XAT	C20-C13-C14	-6.81	113.38	122.92
28	g	619	XAT	C39-C29-C30	-6.81	113.38	122.92
28	Ba	301	XAT	C39-C29-C30	-6.81	113.38	122.92
24	BE	608	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	8	307	CHL	CHD-C1D-ND	-6.81	118.20	124.45
24	BE	604	CLA	C4A-NA-C1A	6.80	109.77	106.71
28	BB	301	XAT	C40-C33-C34	-6.80	113.39	122.92
28	Ba	301	XAT	C6-C7-C8	-6.80	111.61	125.99
24	AA	314	CLA	C4A-NA-C1A	6.80	109.76	106.71
28	BQ	619	XAT	C6-C7-C8	-6.80	111.62	125.99
23	6	609	CHL	C4A-NA-C1A	6.80	109.76	106.71
28	N	619	XAT	C40-C33-C34	-6.79	113.41	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BJ	619	XAT	C40-C33-C34	-6.79	113.41	122.92
24	r	610	CLA	C4A-NA-C1A	6.79	109.76	106.71
28	BJ	619	XAT	C39-C29-C30	-6.79	113.41	122.92
24	6	613	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	n	610	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	N	602	CLA	C4A-NA-C1A	6.78	109.76	106.71
24	S	611	CLA	C4A-NA-C1A	6.78	109.76	106.71
28	n	619	XAT	C6-C7-C8	-6.78	111.65	125.99
28	8	312	XAT	C39-C29-C30	-6.78	113.42	122.92
24	1	504	CLA	C4A-NA-C1A	6.78	109.75	106.71
24	R	404	CLA	C4A-NA-C1A	6.78	109.75	106.71
24	b	604	CLA	C4A-NA-C1A	6.78	109.75	106.71
24	A2	611	CLA	C4A-NA-C1A	6.77	109.75	106.71
24	7	314	CLA	C4A-NA-C1A	6.77	109.75	106.71
28	BQ	619	XAT	C39-C29-C30	-6.77	113.44	122.92
24	C	505	CLA	C4A-NA-C1A	6.76	109.75	106.71
23	6	601	CHL	CHD-C1D-ND	-6.76	118.24	124.45
28	g	619	XAT	C40-C33-C34	-6.76	113.45	122.92
24	n	604	CLA	C4A-NA-C1A	6.76	109.75	106.71
24	a	406	CLA	C4A-NA-C1A	6.76	109.75	106.71
24	A6	610	CLA	C4A-NA-C1A	6.76	109.75	106.71
28	Au	619	XAT	C19-C9-C10	-6.76	113.45	122.92
24	v	612	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	0	604	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	BV	611	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	7	313	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	c	513	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	AB	308	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	Au	612	CLA	C4A-NA-C1A	6.75	109.74	106.71
28	y	301	XAT	C19-C9-C10	-6.75	113.47	122.92
24	C	504	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	1	512	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	BB	305	CLA	C4A-NA-C1A	6.75	109.74	106.71
28	5	619	XAT	C40-C33-C34	-6.75	113.47	122.92
24	Y	305	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	AB	301	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	c	508	CLA	C4A-NA-C1A	6.74	109.74	106.71
28	Ba	301	XAT	C19-C9-C10	-6.74	113.48	122.92
24	BV	610	CLA	C4A-NA-C1A	6.74	109.73	106.71
24	BB	313	CLA	C4A-NA-C1A	6.74	109.73	106.71
24	G	610	CLA	C4A-NA-C1A	6.73	109.73	106.71
24	1	510	CLA	C4A-NA-C1A	6.73	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	301	XAT	C20-C13-C14	-6.73	113.49	122.92
24	G	614	CLA	C4A-NA-C1A	6.73	109.73	106.71
24	BE	615	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	Ba	302	CHL	CHD-C1D-ND	-6.73	118.27	124.45
28	n	619	XAT	C39-C29-C30	-6.73	113.50	122.92
23	n	609	CHL	C2C-C3C-C4C	-6.73	101.69	106.49
23	0	601	CHL	CHD-C1D-ND	-6.73	118.27	124.45
28	BB	301	XAT	C20-C13-C14	-6.73	113.50	122.92
23	y	302	CHL	CHD-C1D-ND	-6.73	118.27	124.45
24	BJ	603	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	7	310	CHL	C2C-C3C-C4C	-6.72	101.70	106.49
28	9	619	XAT	C40-C33-C34	-6.72	113.51	122.92
24	BG	402	CLA	C4A-NA-C1A	6.72	109.73	106.71
28	5	619	XAT	C6-C7-C8	-6.72	111.79	125.99
24	B	610	CLA	C4A-NA-C1A	6.72	109.72	106.71
24	Y	313	CLA	C4A-NA-C1A	6.71	109.72	106.71
24	BU	608	CLA	C4A-NA-C1A	6.71	109.72	106.71
24	B	612	CLA	C4A-NA-C1A	6.71	109.72	106.71
28	G	619	XAT	C19-C9-C10	-6.71	113.52	122.92
24	A6	611	CLA	C4A-NA-C1A	6.71	109.72	106.71
24	1	505	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	BU	606	CHL	CHD-C1D-ND	-6.70	118.30	124.45
24	g	613	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	Au	603	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	s	602	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	S	610	CLA	C4A-NA-C1A	6.69	109.72	106.71
24	Au	602	CLA	C4A-NA-C1A	6.69	109.72	106.71
24	9	611	CLA	C4A-NA-C1A	6.69	109.71	106.71
24	BU	614	CLA	C4A-NA-C1A	6.69	109.71	106.71
28	N	619	XAT	C39-C29-C30	-6.69	113.55	122.92
23	BQ	601	CHL	CHD-C1D-ND	-6.69	118.31	124.45
24	s	610	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	BJ	611	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	5	613	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	y	315	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	BQ	610	CLA	C4A-NA-C1A	6.68	109.71	106.71
28	5	619	XAT	C20-C13-C14	-6.68	113.56	122.92
24	d	402	CLA	C4A-NA-C1A	6.68	109.71	106.71
28	N	619	XAT	C20-C13-C14	-6.67	113.57	122.92
28	y	301	XAT	C40-C33-C34	-6.67	113.57	122.92
24	v	608	CLA	C4A-NA-C1A	6.67	109.71	106.71
24	BE	603	CLA	C4A-NA-C1A	6.67	109.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	y	301	XAT	C20-C13-C14	-6.67	113.58	122.92
24	BB	312	CLA	C4A-NA-C1A	6.67	109.70	106.71
24	BE	607	CLA	C4A-NA-C1A	6.67	109.70	106.71
28	Ba	301	XAT	C40-C33-C34	-6.66	113.59	122.92
24	BV	613	CLA	C4A-NA-C1A	6.66	109.70	106.71
28	AA	301	XAT	C19-C9-C10	-6.66	113.59	122.92
24	C	512	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	5	611	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	BV	609	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	BU	610	CLA	C4A-NA-C1A	6.66	109.70	106.71
28	Ba	301	XAT	C20-C13-C14	-6.66	113.60	122.92
24	g	611	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	AA	306	CHL	CHD-C1D-ND	-6.65	118.34	124.45
23	n	601	CHL	CHD-C1D-ND	-6.65	118.34	124.45
28	g	619	XAT	C18-C5-C6	-6.65	111.11	122.26
28	r	616	XAT	C38-C25-C26	-6.65	111.11	122.26
24	C	506	CLA	C4A-NA-C1A	6.65	109.69	106.71
24	c	504	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	AA	310	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
24	s	609	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	BE	613	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	7	301	XAT	C19-C9-C10	-6.64	113.62	122.92
24	Y	312	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	A	405	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	BJ	619	XAT	C18-C5-C6	-6.64	111.14	122.26
23	y	309	CHL	CHD-C1D-ND	-6.64	118.36	124.45
24	y	303	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	C	510	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	BV	612	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	Ba	315	CLA	C4A-NA-C1A	6.63	109.69	106.71
28	BU	616	XAT	C38-C25-C26	-6.63	111.15	122.26
24	7	311	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	s	613	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	7	306	CHL	CHD-C1D-ND	-6.63	118.36	124.45
24	b	613	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	BJ	613	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	B	601	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	BQ	613	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	G	619	XAT	C39-C29-C30	-6.62	113.65	122.92
24	BQ	604	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	b	608	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	Au	619	XAT	C39-C29-C30	-6.61	113.66	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	r	606	CHL	CHD-C1D-ND	-6.61	118.38	124.45
28	Ba	301	XAT	C38-C25-C26	-6.61	111.18	122.26
24	b	615	CLA	C4A-NA-C1A	6.61	109.68	106.71
24	v	601	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	0	609	CHL	CHD-C1D-ND	-6.61	118.38	124.45
24	AA	313	CLA	C4A-NA-C1A	6.61	109.68	106.71
28	9	619	XAT	C18-C5-C6	-6.61	111.19	122.26
24	9	613	CLA	C4A-NA-C1A	6.60	109.67	106.71
28	G	619	XAT	C18-C5-C6	-6.60	111.19	122.26
23	5	609	CHL	CHB-C1B-NB	-6.60	117.28	124.26
24	n	613	CLA	C4A-NA-C1A	6.60	109.67	106.71
28	AA	318	XAT	C18-C5-C6	-6.59	111.21	122.26
24	BF	504	CLA	C4A-NA-C1A	6.59	109.67	106.71
28	y	301	XAT	C38-C25-C26	-6.59	111.21	122.26
28	Au	619	XAT	C18-C5-C6	-6.59	111.21	122.26
28	8	312	XAT	C38-C25-C26	-6.59	111.22	122.26
24	G	604	CLA	C4A-NA-C1A	6.59	109.67	106.71
28	BQ	619	XAT	C18-C5-C6	-6.59	111.22	122.26
28	AB	312	XAT	C38-C25-C26	-6.58	111.22	122.26
28	7	318	XAT	C19-C9-C10	-6.58	113.70	122.92
24	BE	611	CLA	C4A-NA-C1A	6.58	109.66	106.71
24	8	301	CLA	C4A-NA-C1A	6.58	109.66	106.71
24	B	609	CLA	C4A-NA-C1A	6.58	109.66	106.71
24	R	405	CLA	C4A-NA-C1A	6.58	109.66	106.71
24	7	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
28	n	619	XAT	C18-C5-C6	-6.57	111.25	122.26
24	AA	311	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	A2	614	CLA	C4A-NA-C1A	6.57	109.66	106.71
28	7	318	XAT	C18-C5-C6	-6.57	111.25	122.26
28	y	301	XAT	C18-C5-C6	-6.57	111.25	122.26
24	G	613	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	s	612	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	Au	613	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	BV	602	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	6	605	CHL	CHD-C1D-ND	-6.56	118.42	124.45
24	A	406	CLA	C4A-NA-C1A	6.56	109.66	106.71
24	c	502	CLA	C4A-NA-C1A	6.56	109.66	106.71
28	Ba	301	XAT	C26-C27-C28	-6.56	112.12	125.99
24	N	614	CLA	C4A-NA-C1A	6.56	109.66	106.71
24	g	604	CLA	C4A-NA-C1A	6.56	109.65	106.71
38	A	408	PHO	C4D-CHA-CBD	-6.56	105.55	108.52
28	AA	301	XAT	C18-C5-C6	-6.56	111.27	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	602	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	v	603	CLA	C4A-NA-C1A	6.55	109.65	106.71
28	7	301	XAT	C18-C5-C6	-6.55	111.28	122.26
24	r	611	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	AA	315	CLA	C4A-NA-C1A	6.55	109.65	106.71
38	BD	408	PHO	C4D-CHA-CBD	-6.55	105.55	108.52
28	g	619	XAT	C26-C27-C28	-6.55	112.14	125.99
28	BJ	619	XAT	C20-C13-C14	-6.55	113.75	122.92
23	S	607	CHL	CHD-C1D-ND	-6.55	118.44	124.45
24	B	616	CLA	C4A-NA-C1A	6.54	109.65	106.71
24	b	602	CLA	C4A-NA-C1A	6.54	109.65	106.71
24	v	610	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	0	605	CHL	CHD-C1D-ND	-6.54	118.44	124.45
28	5	619	XAT	C18-C5-C6	-6.54	111.30	122.26
24	BJ	604	CLA	C4A-NA-C1A	6.54	109.65	106.71
24	BF	502	CLA	C4A-NA-C1A	6.54	109.65	106.71
24	BU	612	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	9	605	CHL	CHD-C1D-ND	-6.54	118.45	124.45
24	A6	613	CLA	C4A-NA-C1A	6.54	109.64	106.71
28	BJ	619	XAT	C26-C27-C28	-6.53	112.18	125.99
24	n	614	CLA	C4A-NA-C1A	6.53	109.64	106.71
28	g	619	XAT	C19-C9-C10	-6.53	113.77	122.92
28	BJ	619	XAT	C6-C7-C8	-6.53	112.19	125.99
28	g	619	XAT	C20-C13-C14	-6.53	113.78	122.92
24	B	608	CLA	C4A-NA-C1A	6.53	109.64	106.71
24	v	606	CLA	C4A-NA-C1A	6.53	109.64	106.71
24	1	511	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	BQ	609	CHL	CHD-C1D-ND	-6.53	118.46	124.45
28	BQ	619	XAT	C20-C13-C14	-6.52	113.78	122.92
24	c	505	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	b	607	CLA	C4A-NA-C1A	6.52	109.64	106.71
28	y	301	XAT	C26-C27-C28	-6.52	112.21	125.99
24	BE	612	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	1	506	CLA	C4A-NA-C1A	6.52	109.64	106.71
28	Ba	301	XAT	C18-C5-C6	-6.52	111.33	122.26
28	BJ	619	XAT	C19-C9-C10	-6.52	113.79	122.92
28	Y	301	XAT	C6-C7-C8	-6.52	112.21	125.99
24	S	613	CLA	C4A-NA-C1A	6.51	109.64	106.71
24	b	612	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	Ba	309	CHL	CHD-C1D-ND	-6.51	118.47	124.45
24	A2	610	CLA	C4A-NA-C1A	6.51	109.63	106.71
28	g	619	XAT	C6-C7-C8	-6.51	112.23	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Au	604	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	BU	611	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	BE	602	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	5	612	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	G	612	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	v	605	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	BQ	614	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	5	605	CHL	CHD-C1D-ND	-6.50	118.48	124.45
32	Az	101	SQD	O9-S-C6	6.50	114.66	106.94
23	9	601	CHL	CHD-C1D-ND	-6.49	118.49	124.45
24	6	602	CLA	C4A-NA-C1A	6.49	109.62	106.71
24	8	302	CLA	C4A-NA-C1A	6.49	109.62	106.71
24	B	603	CLA	C4A-NA-C1A	6.49	109.62	106.71
28	BB	301	XAT	C6-C7-C8	-6.49	112.28	125.99
24	Ba	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	Ba	312	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	BQ	603	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	BB	314	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	v	616	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	r	605	CHL	CAC-C3C-C4C	6.48	133.21	124.81
38	a	408	PHO	C4D-CHA-CBD	-6.47	105.59	108.52
38	R	407	PHO	C4D-CHA-CBD	-6.47	105.59	108.52
24	B	605	CLA	C4A-NA-C1A	6.47	109.62	106.71
24	A6	608	CLA	C4A-NA-C1A	6.47	109.62	106.71
28	AA	318	XAT	C19-C9-C10	-6.47	113.86	122.92
24	y	304	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	Au	608	CHL	CHD-C1D-ND	-6.47	118.51	124.45
28	BU	616	XAT	C26-C27-C28	-6.47	112.31	125.99
24	Y	314	CLA	C4A-NA-C1A	6.47	109.61	106.71
24	y	314	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	5	601	CHL	CHD-C1D-ND	-6.46	118.51	124.45
23	A6	606	CHL	O2D-CGD-CBD	6.46	122.75	111.27
28	Y	301	XAT	C38-C25-C26	-6.46	111.43	122.26
24	C	502	CLA	C4A-NA-C1A	6.46	109.61	106.71
28	r	616	XAT	C26-C27-C28	-6.46	112.34	125.99
24	b	603	CLA	C4A-NA-C1A	6.46	109.61	106.71
28	G	619	XAT	C26-C27-C28	-6.46	112.34	125.99
28	Au	619	XAT	C26-C27-C28	-6.46	112.34	125.99
28	N	619	XAT	C26-C27-C28	-6.45	112.35	125.99
24	A	407	CLA	C4A-NA-C1A	6.45	109.61	106.71
28	G	619	XAT	C6-C7-C8	-6.45	112.36	125.99
24	r	612	CLA	C4A-NA-C1A	6.45	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BV	607	CHL	CHD-C1D-ND	-6.44	118.54	124.45
24	n	603	CLA	C4A-NA-C1A	6.44	109.60	106.71
24	Ba	311	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	1	502	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	BJ	602	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	G	608	CHL	CHD-C1D-ND	-6.43	118.55	124.45
23	s	607	CHL	CHD-C1D-ND	-6.43	118.55	124.45
28	N	619	XAT	C6-C7-C8	-6.43	112.40	125.99
23	n	609	CHL	CHD-C1D-ND	-6.43	118.55	124.45
28	9	619	XAT	C6-C7-C8	-6.43	112.41	125.99
24	Ba	314	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	S	606	CHL	O2D-CGD-CBD	6.41	122.66	111.27
24	S	608	CLA	C4A-NA-C1A	6.41	109.59	106.71
24	b	616	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	s	601	CHL	CHD-C1D-ND	-6.41	118.57	124.45
28	Au	619	XAT	C6-C7-C8	-6.41	112.45	125.99
24	y	312	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	0	602	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	1	509	CLA	C4A-NA-C1A	6.40	109.58	106.71
28	7	318	XAT	C6-C7-C8	-6.40	112.47	125.99
28	g	619	XAT	C38-C25-C26	-6.39	111.55	122.26
28	BJ	619	XAT	C38-C25-C26	-6.39	111.55	122.26
24	6	603	CLA	C4A-NA-C1A	6.39	109.58	106.71
24	Ba	304	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	Y	310	CHL	CHD-C1D-ND	-6.39	118.58	124.45
28	n	619	XAT	C38-C25-C26	-6.39	111.55	122.26
24	B	606	CLA	C4A-NA-C1A	6.38	109.58	106.71
24	R	406	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	8	310	CLA	C4A-NA-C1A	6.37	109.57	106.71
23	6	608	CHL	CHD-C1D-ND	-6.37	118.60	124.45
28	AA	318	XAT	C6-C7-C8	-6.36	112.54	125.99
24	8	308	CLA	C4A-NA-C1A	6.36	109.57	106.71
23	BU	605	CHL	CAC-C3C-C4C	6.36	133.06	124.81
24	g	602	CLA	C4A-NA-C1A	6.36	109.56	106.71
24	B	615	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	0	603	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	BE	616	CLA	C4A-NA-C1A	6.35	109.56	106.71
28	BQ	619	XAT	C38-C25-C26	-6.34	111.63	122.26
23	S	607	CHL	CAC-C3C-C4C	6.34	133.03	124.81
24	BG	401	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	BQ	609	CHL	C2C-C3C-C4C	-6.33	101.97	106.49
28	AA	301	XAT	C6-C7-C8	-6.33	112.60	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	G	605	CHL	CHD-C1D-ND	-6.33	118.64	124.45
28	A2	619	XAT	C26-C27-C28	-6.33	112.61	125.99
24	D	401	CLA	C4A-NA-C1A	6.33	109.55	106.71
24	AB	302	CLA	C4A-NA-C1A	6.33	109.55	106.71
24	s	603	CLA	C4A-NA-C1A	6.32	109.55	106.71
23	9	609	CHL	C4A-NA-C1A	6.32	109.55	106.71
24	v	615	CLA	C4A-NA-C1A	6.32	109.55	106.71
24	y	311	CLA	C4A-NA-C1A	6.32	109.55	106.71
28	A2	619	XAT	C6-C7-C8	-6.31	112.65	125.99
24	BU	603	CLA	C4A-NA-C1A	6.31	109.54	106.71
23	y	306	CHL	CHD-C1D-ND	-6.31	118.66	124.45
24	c	510	CLA	C4A-NA-C1A	6.31	109.54	106.71
28	7	301	XAT	C38-C25-C26	-6.30	111.70	122.26
24	C	509	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	8	305	CHL	CHD-C1D-ND	-6.30	118.67	124.45
23	BB	302	CHL	CHD-C1D-ND	-6.29	118.68	124.45
23	Y	302	CHL	CHD-C1D-ND	-6.28	118.68	124.45
24	BV	603	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	Ba	306	CHL	CHD-C1D-ND	-6.28	118.69	124.45
23	BV	601	CHL	CHD-C1D-ND	-6.28	118.69	124.45
23	0	608	CHL	CHD-C1D-ND	-6.27	118.69	124.45
23	AA	309	CHL	CHD-C1D-ND	-6.27	118.69	124.45
23	BQ	607	CHL	CHD-C1D-ND	-6.27	118.69	124.45
23	7	309	CHL	CHD-C1D-ND	-6.27	118.70	124.45
24	s	604	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	8	306	CHL	CHD-C1D-ND	-6.26	118.70	124.45
28	7	301	XAT	C6-C7-C8	-6.26	112.77	125.99
23	A2	609	CHL	CHD-C1D-ND	-6.25	118.71	124.45
23	N	609	CHL	CHD-C1D-ND	-6.25	118.71	124.45
28	BB	301	XAT	C38-C25-C26	-6.25	111.78	122.26
24	Au	611	CLA	C4A-NA-C1A	6.25	109.52	106.71
23	S	606	CHL	CHD-C1D-ND	-6.24	118.72	124.45
23	AB	305	CHL	CHD-C1D-ND	-6.24	118.72	124.45
28	AA	301	XAT	C38-C25-C26	-6.24	111.80	122.26
23	AA	310	CHL	CHB-C1B-NB	-6.24	117.65	124.26
24	AB	309	CLA	C4A-NA-C1A	6.24	109.51	106.71
23	AB	306	CHL	CHD-C1D-ND	-6.24	118.72	124.45
24	c	512	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	9	610	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	BB	310	CHL	CHD-C1D-ND	-6.23	118.73	124.45
24	8	309	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	6	607	CHL	CHD-C1D-ND	-6.23	118.73	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	607	CHL	CHD-C1D-ND	-6.23	118.73	124.45
23	Au	605	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	g	612	CLA	C4A-NA-C1A	6.22	109.50	106.71
24	BJ	612	CLA	C4A-NA-C1A	6.22	109.50	106.71
23	g	601	CHL	CHD-C1D-ND	-6.22	118.74	124.45
23	Au	601	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	BE	606	CLA	C4A-NA-C1A	6.21	109.50	106.71
24	BV	604	CLA	C4A-NA-C1A	6.21	109.50	106.71
28	N	619	XAT	C18-C5-C6	-6.21	111.85	122.26
28	G	619	XAT	C38-C25-C26	-6.21	111.86	122.26
24	BV	608	CLA	C4A-NA-C1A	6.20	109.49	106.71
24	BF	505	CLA	C4A-NA-C1A	6.20	109.49	106.71
23	9	606	CHL	CHD-C1D-ND	-6.19	118.76	124.45
23	A6	606	CHL	CHD-C1D-ND	-6.19	118.76	124.45
24	r	603	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	A6	609	CLA	C4A-NA-C1A	6.19	109.49	106.71
28	N	619	XAT	C38-C25-C26	-6.18	111.90	122.26
23	BQ	606	CHL	CHD-C1D-ND	-6.18	118.78	124.45
24	7	304	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	S	609	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	2	402	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	BQ	602	CLA	C4A-NA-C1A	6.17	109.48	106.71
28	5	619	XAT	C15-C35-C34	-6.17	110.84	123.47
23	BQ	608	CHL	CHD-C1D-ND	-6.16	118.79	124.45
24	BD	405	CLA	C4A-NA-C1A	6.16	109.48	106.71
23	5	609	CHL	CHD-C1D-ND	-6.16	118.79	124.45
23	BJ	601	CHL	CHD-C1D-ND	-6.16	118.79	124.45
24	AA	304	CLA	C4A-NA-C1A	6.16	109.47	106.71
23	Y	306	CHL	CHD-C1D-ND	-6.15	118.80	124.45
28	7	301	XAT	C26-C27-C28	-6.15	112.98	125.99
23	S	605	CHL	CHD-C1D-ND	-6.15	118.80	124.45
24	n	602	CLA	C4A-NA-C1A	6.15	109.47	106.71
28	Y	301	XAT	C18-C5-C6	-6.15	111.95	122.26
28	A2	619	XAT	C18-C5-C6	-6.15	111.95	122.26
23	G	601	CHL	CHD-C1D-ND	-6.14	118.81	124.45
23	9	607	CHL	O2D-CGD-CBD	6.14	122.18	111.27
28	Au	619	XAT	C38-C25-C26	-6.14	111.97	122.26
28	Y	301	XAT	C26-C27-C28	-6.13	113.02	125.99
24	b	606	CLA	C4A-NA-C1A	6.13	109.46	106.71
24	BJ	610	CLA	C4A-NA-C1A	6.13	109.46	106.71
23	7	310	CHL	CHB-C1B-NB	-6.13	117.77	124.26
23	5	606	CHL	CHD-C1D-ND	-6.13	118.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BB	301	XAT	C18-C5-C6	-6.12	112.00	122.26
28	G	619	XAT	C20-C13-C14	-6.12	114.35	122.92
28	AA	301	XAT	C26-C27-C28	-6.11	113.07	125.99
23	5	608	CHL	CHD-C1D-ND	-6.11	118.84	124.45
23	A6	605	CHL	CHD-C1D-ND	-6.10	118.84	124.45
23	BB	306	CHL	CHD-C1D-ND	-6.10	118.84	124.45
24	d	401	CLA	C4A-NA-C1A	6.10	109.45	106.71
23	g	609	CHL	CHB-C1B-NB	-6.10	117.80	124.26
24	0	614	CLA	C4A-NA-C1A	6.10	109.45	106.71
23	A2	606	CHL	CHD-C1D-ND	-6.10	118.85	124.45
23	BB	309	CHL	CHD-C1D-ND	-6.10	118.85	124.45
24	g	610	CLA	C4A-NA-C1A	6.10	109.45	106.71
23	n	608	CHL	CHD-C1D-ND	-6.10	118.85	124.45
23	n	606	CHL	CHD-C1D-ND	-6.10	118.85	124.45
23	N	606	CHL	CHD-C1D-ND	-6.09	118.86	124.45
23	BJ	609	CHL	CHB-C1B-NB	-6.09	117.81	124.26
23	0	609	CHL	C4A-NA-C1A	6.08	109.44	106.71
24	6	614	CLA	C4A-NA-C1A	6.07	109.44	106.71
23	0	607	CHL	CHD-C1D-ND	-6.07	118.87	124.45
24	AB	310	CLA	C4A-NA-C1A	6.07	109.44	106.71
23	9	608	CHL	CHD-C1D-ND	-6.07	118.87	124.45
23	A2	608	CHL	CHD-C1D-ND	-6.07	118.88	124.45
24	9	602	CLA	C4A-NA-C1A	6.07	109.43	106.71
23	y	308	CHL	CHD-C1D-ND	-6.07	118.88	124.45
24	s	608	CLA	C4A-NA-C1A	6.06	109.43	106.71
23	AB	304	CHL	CHD-C1D-ND	-6.06	118.88	124.45
28	Au	619	XAT	C20-C13-C14	-6.06	114.43	122.92
28	A2	619	XAT	C38-C25-C26	-6.06	112.11	122.26
23	A6	607	CHL	CHB-C1B-NB	-6.05	117.85	124.26
23	8	304	CHL	CHD-C1D-ND	-6.05	118.89	124.45
23	Y	309	CHL	CHD-C1D-ND	-6.05	118.90	124.45
23	g	605	CHL	CHD-C1D-ND	-6.05	118.90	124.45
23	N	601	CHL	CHD-C1D-ND	-6.04	118.90	124.45
28	BB	301	XAT	C26-C27-C28	-6.04	113.23	125.99
23	Ba	308	CHL	CHD-C1D-ND	-6.04	118.91	124.45
23	S	601	CHL	CHD-C1D-ND	-6.03	118.91	124.45
23	N	608	CHL	CHD-C1D-ND	-6.02	118.92	124.45
24	9	603	CLA	C4A-NA-C1A	6.02	109.41	106.71
23	A2	601	CHL	CHD-C1D-ND	-6.02	118.92	124.45
23	n	605	CHL	CHD-C1D-ND	-6.00	118.94	124.45
23	BJ	605	CHL	CHD-C1D-ND	-6.00	118.94	124.45
24	BF	510	CLA	C4A-NA-C1A	5.99	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A6	601	CHL	CHD-C1D-ND	-5.99	118.95	124.45
23	9	609	CHL	CHD-C1D-ND	-5.98	118.95	124.45
23	Y	307	CHL	C3C-C4C-NC	5.98	117.27	110.57
23	BU	605	CHL	CHD-C1D-ND	-5.97	118.97	124.45
23	N	607	CHL	CHD-C1D-ND	-5.96	118.97	124.45
23	s	605	CHL	CHD-C1D-ND	-5.96	118.97	124.45
23	BQ	605	CHL	CHD-C1D-ND	-5.96	118.97	124.45
23	A2	607	CHL	CHD-C1D-ND	-5.96	118.97	124.45
23	9	609	CHL	O2D-CGD-CBD	5.96	121.86	111.27
24	a	405	CLA	C4A-NA-C1A	5.96	109.38	106.71
23	BB	307	CHL	C3C-C4C-NC	5.94	117.23	110.57
23	5	609	CHL	C3B-C2B-C1B	-5.93	100.00	107.16
23	g	608	CHL	CHD-C1D-ND	-5.93	119.01	124.45
23	5	609	CHL	O2D-CGD-CBD	5.92	121.79	111.27
23	Au	607	CHL	CHD-C1D-ND	-5.92	119.02	124.45
23	BJ	607	CHL	CHD-C1D-ND	-5.92	119.02	124.45
23	AA	310	CHL	O2D-CGD-CBD	5.91	121.77	111.27
23	Ba	307	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	7	305	CLA	C4A-NA-C1A	5.90	109.36	106.71
24	G	611	CLA	C4A-NA-C1A	5.90	109.36	106.71
24	AA	305	CLA	C4A-NA-C1A	5.90	109.36	106.71
23	y	307	CHL	CHD-C1D-ND	-5.89	119.04	124.45
23	r	605	CHL	CHD-C1D-ND	-5.89	119.04	124.45
23	g	607	CHL	CHD-C1D-ND	-5.89	119.04	124.45
23	7	310	CHL	O2D-CGD-CBD	5.89	121.73	111.27
23	G	607	CHL	CHD-C1D-ND	-5.89	119.05	124.45
23	BV	606	CHL	CHD-C1D-ND	-5.87	119.06	124.45
23	s	606	CHL	CHD-C1D-ND	-5.87	119.06	124.45
23	Ba	308	CHL	C3B-C2B-C1B	-5.86	100.08	107.16
23	g	606	CHL	CHD-C1D-ND	-5.86	119.07	124.45
23	y	308	CHL	C3B-C2B-C1B	-5.85	100.10	107.16
23	5	606	CHL	C3B-C2B-C1B	-5.84	100.11	107.16
23	0	609	CHL	C3B-C2B-C1B	-5.83	100.12	107.16
23	BJ	608	CHL	CHD-C1D-ND	-5.80	119.12	124.45
23	BJ	606	CHL	CHD-C1D-ND	-5.80	119.12	124.45
23	Au	609	CHL	CHD-C1D-ND	-5.80	119.12	124.45
23	G	607	CHL	C3B-C2B-C1B	-5.80	100.16	107.16
23	N	605	CHL	CHD-C1D-ND	-5.80	119.13	124.45
23	BV	605	CHL	CHD-C1D-ND	-5.80	119.13	124.45
24	5	610	CLA	C4A-NA-C1A	5.79	109.31	106.71
23	g	607	CHL	C3B-C2B-C1B	-5.79	100.17	107.16
23	BJ	607	CHL	C3B-C2B-C1B	-5.79	100.17	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ba	310	CHL	CHB-C1B-NB	-5.77	118.15	124.26
23	AA	308	CHL	C3B-C2B-C1B	-5.77	100.20	107.16
23	7	308	CHL	C3B-C2B-C1B	-5.76	100.20	107.16
23	7	308	CHL	CHD-C1D-ND	-5.76	119.16	124.45
23	A2	605	CHL	CHD-C1D-ND	-5.74	119.18	124.45
23	5	607	CHL	O2D-CGD-CBD	5.74	121.46	111.27
23	9	606	CHL	C3B-C2B-C1B	-5.73	100.24	107.16
23	5	607	CHL	CHD-C1D-ND	-5.73	119.19	124.45
23	AA	308	CHL	CHD-C1D-ND	-5.73	119.19	124.45
23	BQ	607	CHL	C3B-C2B-C1B	-5.71	100.27	107.16
24	5	603	CLA	C4A-NA-C1A	5.71	109.27	106.71
23	A6	607	CHL	C3B-C2B-C1B	-5.71	100.27	107.16
23	7	307	CHL	CHD-C1D-ND	-5.70	119.22	124.45
23	G	606	CHL	CHD-C1D-ND	-5.70	119.22	124.45
23	BB	308	CHL	CHD-C1D-ND	-5.70	119.22	124.45
24	0	610	CLA	C4A-NA-C1A	5.69	109.26	106.71
23	n	607	CHL	C3B-C2B-C1B	-5.68	100.31	107.16
24	9	604	CLA	C4A-NA-C1A	5.68	109.26	106.71
28	BU	616	XAT	C15-C35-C34	-5.67	111.85	123.47
23	r	607	CHL	CHD-C1D-ND	-5.66	119.25	124.45
23	y	309	CHL	CHB-C1B-NB	-5.66	118.26	124.26
23	A2	609	CHL	C3B-C2B-C1B	-5.65	100.34	107.16
23	Au	606	CHL	CHD-C1D-ND	-5.65	119.27	124.45
23	G	609	CHL	C3B-C2B-C1B	-5.65	100.35	107.16
23	BH	601	CHL	CHD-C1D-ND	-5.64	119.27	124.45
23	AA	307	CHL	CHD-C1D-ND	-5.63	119.28	124.45
28	r	616	XAT	C15-C35-C34	-5.63	111.95	123.47
23	e	601	CHL	CHD-C1D-ND	-5.62	119.29	124.45
23	Y	307	CHL	CHD-C1D-ND	-5.61	119.30	124.45
23	BB	307	CHL	CHD-C1D-ND	-5.61	119.30	124.45
23	BU	607	CHL	CHD-C1D-ND	-5.60	119.30	124.45
28	AA	318	XAT	C15-C35-C34	-5.60	112.01	123.47
23	6	609	CHL	C3B-C2B-C1B	-5.60	100.41	107.16
23	9	605	CHL	C3B-C2B-C1B	-5.59	100.41	107.16
28	Au	619	XAT	C15-C35-C34	-5.59	112.02	123.47
23	y	310	CHL	CHB-C1B-NB	-5.59	118.34	124.26
23	8	304	CHL	C3B-C2B-C1B	-5.59	100.42	107.16
23	AB	304	CHL	C3B-C2B-C1B	-5.59	100.42	107.16
35	a	402	BCT	O2-C-O1	5.59	134.03	119.55
24	5	604	CLA	C4A-NA-C1A	5.59	109.22	106.71
23	5	605	CHL	C3B-C2B-C1B	-5.58	100.42	107.16
23	Ba	309	CHL	CHB-C1B-NB	-5.58	118.35	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	609	CHL	C3B-C2B-C1B	-5.58	100.42	107.16
23	0	606	CHL	C3C-C4C-NC	5.58	116.83	110.57
23	e	601	CHL	C3B-C2B-C1B	-5.58	100.43	107.16
23	9	609	CHL	C3B-C2B-C1B	-5.58	100.43	107.16
23	S	607	CHL	C3B-C2B-C1B	-5.58	100.43	107.16
23	AA	310	CHL	C3B-C2B-C1B	-5.57	100.44	107.16
28	7	318	XAT	C15-C35-C34	-5.56	112.09	123.47
35	BD	402	BCT	O2-C-O1	5.55	133.95	119.55
23	Y	308	CHL	CHD-C1D-ND	-5.55	119.36	124.45
28	G	619	XAT	C15-C35-C34	-5.54	112.12	123.47
23	7	310	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
23	G	601	CHL	O2D-CGD-CBD	5.53	121.10	111.27
23	Y	306	CHL	C3B-C2B-C1B	-5.53	100.48	107.16
23	BB	306	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
23	BU	606	CHL	CHB-C1B-NB	-5.53	118.40	124.26
23	0	608	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
23	BH	601	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
23	6	606	CHL	CHD-C1D-ND	-5.52	119.38	124.45
23	Au	607	CHL	C3B-C2B-C1B	-5.52	100.50	107.16
23	5	608	CHL	C3B-C2B-C1B	-5.52	100.50	107.16
23	9	608	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
28	n	619	XAT	C15-C35-C34	-5.51	112.19	123.47
23	A2	606	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
23	BJ	606	CHL	C3B-C2B-C1B	-5.50	100.52	107.16
23	9	607	CHL	CHD-C1D-ND	-5.50	119.40	124.45
23	6	606	CHL	C3C-C4C-NC	5.50	116.74	110.57
23	AA	306	CHL	CHB-C1B-NB	-5.49	118.44	124.26
24	6	610	CLA	CMA-C3A-C4A	-5.49	97.01	111.77
23	r	606	CHL	C3B-C2B-C1B	-5.49	100.53	107.16
23	S	606	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
23	7	306	CHL	CHB-C1B-NB	-5.49	118.45	124.26
23	BJ	605	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
23	Au	609	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
23	6	605	CHL	C3B-C2B-C1B	-5.48	100.54	107.16
23	0	606	CHL	CHD-C1D-ND	-5.48	119.42	124.45
28	BQ	619	XAT	C15-C35-C34	-5.48	112.25	123.47
23	N	606	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
23	BU	606	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
23	r	606	CHL	CHB-C1B-NB	-5.47	118.47	124.26
23	g	605	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
23	g	606	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
23	AA	307	CHL	C3B-C2B-C1B	-5.47	100.56	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	608	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
23	0	605	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
23	A6	606	CHL	C3B-C2B-C1B	-5.45	100.59	107.16
23	7	309	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
23	n	605	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
23	G	606	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
23	7	307	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
23	BQ	605	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
28	AA	301	XAT	C15-C35-C34	-5.43	112.34	123.47
23	G	608	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
23	g	608	CHL	O2D-CGD-CBD	5.42	120.91	111.27
23	n	609	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
23	0	606	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
28	7	301	XAT	C15-C35-C34	-5.42	112.38	123.47
23	AB	305	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
28	Y	301	XAT	C15-C35-C34	-5.41	112.38	123.47
23	Au	605	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
28	BB	301	XAT	C15-C35-C34	-5.41	112.39	123.47
23	AA	309	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
23	5	601	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
23	Ba	309	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
28	A2	619	XAT	O24-C25-C38	-5.40	108.58	115.06
23	r	605	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
23	9	607	CHL	C3C-C4C-NC	5.40	116.63	110.57
23	y	309	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
23	8	306	CHL	CHB-C1B-NB	-5.40	118.54	124.26
23	8	305	CHL	C3B-C2B-C1B	-5.40	100.65	107.16
28	9	619	XAT	C15-C35-C34	-5.40	112.42	123.47
28	BU	616	XAT	C35-C15-C14	-5.39	112.43	123.47
23	BU	607	CHL	C3C-C4C-NC	5.39	116.62	110.57
23	9	601	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
23	G	605	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
23	y	306	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
23	Au	608	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
28	A2	619	XAT	C15-C35-C34	-5.39	112.44	123.47
23	0	609	CHL	C3C-C4C-NC	5.38	116.61	110.57
23	BJ	608	CHL	O2D-CGD-CBD	5.38	120.83	111.27
23	N	601	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
28	y	301	XAT	C15-C35-C34	-5.38	112.46	123.47
23	A2	608	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
35	A	401	BCT	O2-C-O1	5.38	133.49	119.55
23	n	608	CHL	C3B-C2B-C1B	-5.37	100.67	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	605	CHL	C3C-C4C-NC	5.37	116.60	110.57
23	AA	302	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
23	6	607	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
23	s	607	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
23	N	608	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
28	Ba	301	XAT	C15-C35-C34	-5.36	112.49	123.47
23	S	601	CHL	O2D-CGD-CBD	5.36	120.79	111.27
23	Au	601	CHL	O2D-CGD-CBD	5.36	120.79	111.27
23	Ba	306	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
23	BU	605	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
23	AA	306	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
23	A2	601	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
23	6	606	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
23	7	302	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
23	n	606	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
23	BV	607	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
23	n	605	CHL	C3C-C4C-NC	5.34	116.56	110.57
28	N	619	XAT	C15-C35-C34	-5.34	112.53	123.47
23	BV	606	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
23	BB	308	CHL	C3C-C4C-NC	5.34	116.56	110.57
23	A6	601	CHL	O2D-CGD-CBD	5.34	120.75	111.27
23	S	605	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
23	A6	605	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
28	8	312	XAT	C35-C15-C14	-5.34	112.54	123.47
23	BQ	606	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
23	s	606	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
23	BJ	607	CHL	C3C-C4C-NC	5.33	116.55	110.57
23	Y	310	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	BB	302	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	g	601	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	y	310	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
28	A2	619	XAT	C11-C12-C13	-5.33	111.45	126.42
23	6	608	CHL	CHB-C1B-NB	-5.33	118.62	124.26
23	s	606	CHL	C3C-C4C-NC	5.33	116.55	110.57
23	Ba	307	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	A2	607	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	BB	310	CHL	C3B-C2B-C1B	-5.32	100.73	107.16
23	N	605	CHL	C3C-C4C-NC	5.32	116.54	110.57
23	N	607	CHL	C3B-C2B-C1B	-5.32	100.73	107.16
28	AB	312	XAT	C15-C35-C34	-5.32	112.57	123.47
23	r	607	CHL	C3C-C4C-NC	5.32	116.54	110.57
23	BV	606	CHL	C3C-C4C-NC	5.32	116.54	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Au	619	XAT	C11-C12-C13	-5.32	111.48	126.42
23	BQ	609	CHL	C3B-C2B-C1B	-5.32	100.75	107.16
23	s	601	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
23	AB	307	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
35	2	401	BCT	O2-C-O1	5.31	133.33	119.55
23	7	306	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
23	Ba	302	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
23	AB	306	CHL	CHB-C1B-NB	-5.31	118.63	124.26
23	Y	308	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
23	y	302	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
23	A2	607	CHL	C3C-C4C-NC	5.31	116.53	110.57
23	5	601	CHL	CAC-C3C-C4C	5.31	131.70	124.81
28	8	312	XAT	C15-C35-C34	-5.31	112.60	123.47
23	Y	308	CHL	C3C-C4C-NC	5.31	116.52	110.57
23	g	606	CHL	C3C-C4C-NC	5.31	116.52	110.57
28	G	619	XAT	C11-C12-C13	-5.31	111.51	126.42
23	BQ	605	CHL	C3C-C4C-NC	5.30	116.52	110.57
23	BJ	601	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
23	0	608	CHL	CHB-C1B-NB	-5.30	118.64	124.26
23	Y	309	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
23	A6	605	CHL	C3C-C4C-NC	5.30	116.51	110.57
23	n	601	CHL	C3B-C2B-C1B	-5.30	100.77	107.16
23	S	605	CHL	C3C-C4C-NC	5.29	116.51	110.57
23	y	307	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
23	BQ	608	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
23	g	601	CHL	O2D-CGD-CBD	5.29	120.67	111.27
23	BV	601	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
23	Ba	310	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
23	BU	607	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
28	AB	312	XAT	C35-C15-C14	-5.29	112.64	123.47
23	N	605	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
23	0	607	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
23	BQ	601	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
23	Y	302	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
23	BB	308	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
23	BB	309	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
23	Au	606	CHL	C3B-C2B-C1B	-5.27	100.79	107.16
23	BJ	606	CHL	C3C-C4C-NC	5.27	116.48	110.57
28	r	616	XAT	C35-C15-C14	-5.27	112.68	123.47
23	r	607	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
28	N	619	XAT	C11-C12-C13	-5.27	111.62	126.42
23	5	606	CHL	C3C-C4C-NC	5.27	116.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	605	CHL	C3C-C4C-NC	5.27	116.48	110.57
23	Y	307	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
23	6	605	CHL	CHB-C1B-NB	-5.26	118.69	124.26
25	7	316	LUT	C35-C15-C14	5.26	134.25	123.47
23	g	607	CHL	C3C-C4C-NC	5.26	116.47	110.57
31	BG	403	PL9	C7-C3-C4	5.26	121.15	116.88
23	Au	607	CHL	C3C-C4C-NC	5.26	116.47	110.57
23	A6	601	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
23	y	307	CHL	C3C-C4C-NC	5.25	116.46	110.57
23	Ba	307	CHL	C3C-C4C-NC	5.25	116.46	110.57
28	9	619	XAT	C35-C15-C14	-5.25	112.71	123.47
31	d	403	PL9	C7-C3-C4	5.25	121.14	116.88
23	BJ	601	CHL	O2D-CGD-CBD	5.25	120.60	111.27
23	0	605	CHL	CHB-C1B-NB	-5.25	118.70	124.26
23	9	601	CHL	CAC-C3C-C4C	5.24	131.61	124.81
23	N	607	CHL	C3C-C4C-NC	5.24	116.44	110.57
23	g	605	CHL	C3C-C4C-NC	5.24	116.44	110.57
24	b	611	CLA	CMC-C2C-C1C	-5.23	117.07	125.04
23	AA	308	CHL	C3C-C4C-NC	5.23	116.43	110.57
23	BB	307	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
23	Ba	308	CHL	C3C-C4C-NC	5.22	116.42	110.57
23	S	601	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
23	8	307	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
28	Y	301	XAT	C11-C12-C13	-5.21	111.77	126.42
28	BB	301	XAT	C11-C12-C13	-5.21	111.77	126.42
23	g	609	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
23	A2	606	CHL	C3C-C4C-NC	5.21	116.41	110.57
23	G	607	CHL	C3C-C4C-NC	5.21	116.41	110.57
23	Au	606	CHL	C3C-C4C-NC	5.20	116.41	110.57
23	7	308	CHL	C3C-C4C-NC	5.20	116.40	110.57
23	BU	607	CHL	O2D-CGD-CBD	5.19	120.50	111.27
23	G	606	CHL	C3C-C4C-NC	5.19	116.39	110.57
28	y	301	XAT	C11-C12-C13	-5.18	111.85	126.42
23	s	601	CHL	O2D-CGD-CBD	5.18	120.47	111.27
23	9	606	CHL	C3C-C4C-NC	5.18	116.38	110.57
23	BJ	609	CHL	C3B-C2B-C1B	-5.18	100.91	107.16
28	Ba	301	XAT	C11-C12-C13	-5.17	111.88	126.42
23	A2	605	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
23	BJ	608	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
23	g	608	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
23	BU	605	CHL	C1C-C2C-C3C	-5.17	103.01	107.11
23	8	306	CHL	C3B-C2B-C1B	-5.16	100.93	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	601	CHL	C3C-C4C-NC	5.16	116.36	110.57
23	AB	304	CHL	CHB-C1B-NB	-5.16	118.80	124.26
23	AB	306	CHL	C3B-C2B-C1B	-5.15	100.94	107.16
23	Ba	310	CHL	C4A-NA-C1A	5.15	109.02	106.71
28	y	301	XAT	C8-C9-C10	-5.15	111.03	118.94
28	N	619	XAT	O24-C25-C38	-5.15	108.88	115.06
23	5	605	CHL	CHB-C1B-NB	-5.15	118.80	124.26
23	N	608	CHL	CHB-C1B-NB	-5.15	118.80	124.26
24	6	610	CLA	C4A-NA-C1A	5.15	109.02	106.71
28	AB	312	XAT	C12-C13-C14	-5.15	111.04	118.94
23	BB	306	CHL	CHB-C1B-NB	-5.15	118.81	124.26
23	G	605	CHL	C3C-C4C-NC	5.14	116.34	110.57
23	r	613	CHL	C3B-C2B-C1B	-5.14	100.95	107.16
23	A2	609	CHL	C3C-C4C-NC	5.14	116.34	110.57
23	Y	306	CHL	CHB-C1B-NB	-5.14	118.82	124.26
23	9	605	CHL	CHB-C1B-NB	-5.14	118.82	124.26
28	Ba	301	XAT	C8-C9-C10	-5.14	111.06	118.94
23	A2	608	CHL	CHB-C1B-NB	-5.13	118.82	124.26
23	G	601	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
23	n	607	CHL	C3C-C4C-NC	5.13	116.32	110.57
23	BH	601	CHL	C3C-C4C-NC	5.12	116.32	110.57
23	BQ	608	CHL	CHB-C1B-NB	-5.12	118.83	124.26
23	g	601	CHL	C3C-C4C-NC	5.12	116.31	110.57
23	e	601	CHL	C3C-C4C-NC	5.12	116.31	110.57
23	y	308	CHL	C3C-C4C-NC	5.12	116.31	110.57
23	BQ	607	CHL	C3C-C4C-NC	5.12	116.31	110.57
23	r	607	CHL	O2D-CGD-CBD	5.12	120.36	111.27
28	8	312	XAT	C12-C13-C14	-5.11	111.10	118.94
23	G	605	CHL	O2D-CGD-CBD	5.11	120.34	111.27
24	BV	604	CLA	C3B-C4B-NB	-5.10	105.78	110.52
28	g	619	XAT	C15-C35-C34	-5.10	113.02	123.47
23	n	608	CHL	CHB-C1B-NB	-5.10	118.86	124.26
23	5	607	CHL	C3C-C4C-NC	5.10	116.29	110.57
28	y	301	XAT	C35-C15-C14	-5.10	113.03	123.47
23	5	609	CHL	C3C-C4C-NC	5.10	116.29	110.57
28	BJ	619	XAT	C15-C35-C34	-5.09	113.04	123.47
23	s	607	CHL	CHB-C1B-NB	-5.09	118.87	124.26
23	Au	605	CHL	O2D-CGD-CBD	5.09	120.31	111.27
28	5	619	XAT	C11-C12-C13	-5.08	112.13	126.42
23	9	601	CHL	C3C-C4C-NC	5.08	116.27	110.57
23	5	607	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
23	9	607	CHL	C3B-C2B-C1B	-5.07	101.04	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Au	601	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
23	N	606	CHL	C3C-C4C-NC	5.07	116.26	110.57
23	S	607	CHL	C3C-C4C-NC	5.07	116.26	110.57
23	BV	601	CHL	O2D-CGD-CBD	5.07	120.27	111.27
28	Ba	301	XAT	C35-C15-C14	-5.06	113.10	123.47
23	BV	605	CHL	C3B-C2B-C1B	-5.06	101.05	107.16
23	0	601	CHL	C3C-C4C-NC	5.06	116.25	110.57
23	6	601	CHL	C3B-C2B-C1B	-5.06	101.06	107.16
28	7	318	XAT	C35-C15-C14	-5.06	113.11	123.47
23	BV	607	CHL	CHB-C1B-NB	-5.06	118.91	124.26
28	BQ	619	XAT	C11-C12-C13	-5.05	112.23	126.42
28	g	619	XAT	C35-C15-C14	-5.05	113.13	123.47
23	5	609	CHL	C4A-NA-C1A	5.05	108.98	106.71
23	N	609	CHL	C3C-C4C-NC	5.05	116.23	110.57
23	7	307	CHL	C3C-C4C-NC	5.04	116.23	110.57
28	BJ	619	XAT	C35-C15-C14	-5.04	113.15	123.47
28	n	619	XAT	C35-C15-C14	-5.04	113.16	123.47
23	AA	307	CHL	C3C-C4C-NC	5.03	116.21	110.57
23	7	302	CHL	O2D-CGD-CBD	5.03	120.20	111.27
28	AA	301	XAT	O24-C25-C38	-5.03	109.03	115.06
23	5	601	CHL	C3C-C4C-NC	5.03	116.21	110.57
23	n	606	CHL	C3C-C4C-NC	5.03	116.21	110.57
23	Au	609	CHL	C3C-C4C-NC	5.03	116.21	110.57
23	S	606	CHL	C3C-C4C-NC	5.02	116.20	110.57
23	BU	613	CHL	C3B-C2B-C1B	-5.02	101.10	107.16
23	A6	606	CHL	C3C-C4C-NC	5.02	116.20	110.57
23	Au	605	CHL	C3C-C4C-NC	5.01	116.19	110.57
28	9	619	XAT	C31-C32-C33	-5.01	112.35	126.42
28	AA	318	XAT	C35-C15-C14	-5.01	113.22	123.47
23	s	605	CHL	C3B-C2B-C1B	-5.00	101.12	107.16
23	BB	310	CHL	C3C-C4C-NC	5.00	116.17	110.57
23	Y	302	CHL	O2D-CGD-CBD	4.99	120.14	111.27
23	6	609	CHL	C3C-C4C-NC	4.99	116.16	110.57
28	BQ	619	XAT	C35-C15-C14	-4.99	113.26	123.47
23	8	304	CHL	CHB-C1B-NB	-4.98	118.98	124.26
28	5	619	XAT	C35-C15-C14	-4.98	113.28	123.47
28	AB	312	XAT	O4-C5-C18	-4.98	109.09	115.06
23	BB	310	CHL	O2D-CGD-CBD	4.97	120.11	111.27
23	BV	605	CHL	O2D-CGD-CBD	4.97	120.11	111.27
23	0	601	CHL	C3B-C2B-C1B	-4.97	101.16	107.16
25	Au	615	LUT	C15-C35-C34	4.97	133.66	123.47
23	BV	605	CHL	C3C-C4C-NC	4.97	116.15	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	608	CHL	C3C-C4C-NC	4.96	116.14	110.57
23	9	609	CHL	C3C-C4C-NC	4.96	116.14	110.57
23	BB	302	CHL	O2D-CGD-CBD	4.96	120.09	111.27
23	5	606	CHL	O2D-CGD-CBD	4.96	120.08	111.27
23	BB	307	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
23	Y	307	CHL	CHD-C4C-C3C	-4.96	117.55	124.84
23	G	609	CHL	CHB-C1B-NB	-4.96	119.01	124.26
23	6	601	CHL	C3C-C4C-NC	4.95	116.12	110.57
23	s	605	CHL	O2D-CGD-CBD	4.95	120.07	111.27
23	Y	307	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
23	BB	309	CHL	C3C-C4C-NC	4.95	116.12	110.57
23	Ba	302	CHL	O2D-CGD-CBD	4.94	120.05	111.27
23	r	613	CHL	O2D-CGD-CBD	4.94	120.05	111.27
23	g	608	CHL	C3C-C4C-NC	4.94	116.11	110.57
23	9	606	CHL	O2D-CGD-CBD	4.94	120.05	111.27
28	5	619	XAT	C32-C33-C34	-4.94	111.36	118.94
23	N	601	CHL	C3C-C4C-NC	4.94	116.11	110.57
23	BB	307	CHL	CHD-C4C-C3C	-4.94	117.59	124.84
28	9	619	XAT	C11-C12-C13	-4.93	112.55	126.42
28	7	301	XAT	O24-C25-C38	-4.93	109.15	115.06
25	G	615	LUT	C15-C35-C34	4.93	133.57	123.47
23	BB	302	CHL	C3C-C4C-NC	4.93	116.10	110.57
28	8	312	XAT	O4-C5-C18	-4.92	109.16	115.06
28	n	619	XAT	C11-C12-C13	-4.92	112.58	126.42
28	BQ	619	XAT	C8-C9-C10	-4.92	111.39	118.94
23	S	607	CHL	CHB-C1B-NB	-4.92	119.05	124.26
23	BQ	606	CHL	CHB-C1B-NB	-4.92	119.05	124.26
23	BU	606	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
23	Y	309	CHL	C3C-C4C-NC	4.92	116.08	110.57
23	Y	302	CHL	C3C-C4C-NC	4.91	116.07	110.57
23	A2	601	CHL	C3C-C4C-NC	4.90	116.06	110.57
25	BJ	616	LUT	C19-C9-C10	-4.90	116.06	122.92
23	y	302	CHL	O2D-CGD-CBD	4.90	119.97	111.27
23	BU	613	CHL	C3C-C4C-NC	4.89	116.06	110.57
23	S	607	CHL	OMC-CMC-C2C	-4.89	114.62	125.69
28	BB	301	XAT	O24-C25-C38	-4.89	109.20	115.06
23	r	606	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
23	7	309	CHL	C3C-C4C-NC	4.88	116.05	110.57
28	7	318	XAT	C11-C12-C13	-4.88	112.70	126.42
23	G	601	CHL	C3C-C4C-NC	4.88	116.05	110.57
23	Y	310	CHL	C3C-C4C-NC	4.88	116.05	110.57
23	8	307	CHL	O2D-CGD-CBD	4.88	119.94	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	AA	318	XAT	C11-C12-C13	-4.88	112.72	126.42
23	s	605	CHL	C3C-C4C-NC	4.87	116.04	110.57
23	r	607	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
28	G	619	XAT	O24-C25-C38	-4.87	109.22	115.06
28	n	619	XAT	C8-C9-C10	-4.87	111.47	118.94
23	AA	309	CHL	C3C-C4C-NC	4.86	116.03	110.57
23	0	608	CHL	C3C-C4C-NC	4.86	116.03	110.57
23	S	605	CHL	O2D-CGD-CBD	4.86	119.91	111.27
28	Au	619	XAT	O24-C25-C38	-4.86	109.23	115.06
23	S	601	CHL	C3C-C4C-NC	4.86	116.02	110.57
23	A6	605	CHL	O2D-CGD-CBD	4.85	119.89	111.27
23	BQ	601	CHL	C3C-C4C-NC	4.85	116.00	110.57
23	BV	601	CHL	C3C-C4C-NC	4.85	116.00	110.57
23	5	601	CHL	C3D-C2D-C1D	-4.84	99.22	105.83
23	9	601	CHL	C3D-C2D-C1D	-4.84	99.22	105.83
28	g	619	XAT	C11-C12-C13	-4.84	112.81	126.42
23	AA	302	CHL	C3C-C4C-NC	4.84	116.00	110.57
28	BJ	619	XAT	C11-C12-C13	-4.83	112.85	126.42
23	n	601	CHL	C3C-C4C-NC	4.83	115.99	110.57
23	y	306	CHL	C3C-C4C-NC	4.82	115.98	110.57
23	BQ	606	CHL	C3C-C4C-NC	4.82	115.98	110.57
23	s	601	CHL	C3C-C4C-NC	4.82	115.98	110.57
23	S	607	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
23	BU	607	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
23	AB	305	CHL	C3C-C4C-NC	4.82	115.97	110.57
28	BB	301	XAT	C38-C25-C24	-4.81	108.86	114.28
23	8	305	CHL	C3C-C4C-NC	4.81	115.97	110.57
23	Ba	302	CHL	C3C-C4C-NC	4.81	115.97	110.57
23	n	608	CHL	C3C-C4C-NC	4.81	115.96	110.57
23	Ba	306	CHL	C3C-C4C-NC	4.81	115.96	110.57
28	7	318	XAT	C31-C32-C33	-4.81	112.91	126.42
28	AA	318	XAT	C31-C32-C33	-4.81	112.91	126.42
23	AA	302	CHL	O2D-CGD-CBD	4.81	119.81	111.27
28	r	616	XAT	C12-C13-C14	-4.80	111.57	118.94
23	9	608	CHL	CHB-C1B-NB	-4.80	119.18	124.26
23	BQ	608	CHL	C3C-C4C-NC	4.80	115.95	110.57
23	5	608	CHL	CHB-C1B-NB	-4.80	119.18	124.26
23	A6	607	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
23	AA	302	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
23	Y	306	CHL	C3C-C4C-NC	4.79	115.94	110.57
23	7	302	CHL	C3D-C2D-C1D	-4.78	99.30	105.83
28	AA	301	XAT	C11-C12-C13	-4.78	112.98	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	y	302	CHL	C3C-C4C-NC	4.78	115.93	110.57
23	7	302	CHL	C3C-C4C-NC	4.78	115.93	110.57
23	Ba	307	CHL	CHB-C1B-NB	-4.78	119.20	124.26
28	7	301	XAT	C11-C12-C13	-4.78	112.99	126.42
32	Az	101	SQD	O7-S-C6	4.78	112.61	106.94
32	Az	101	SQD	O9-S-O7	-4.77	97.42	113.95
23	0	608	CHL	O2D-CGD-CBD	4.77	119.74	111.27
23	6	608	CHL	C3C-C4C-NC	4.77	115.92	110.57
23	A6	601	CHL	C3C-C4C-NC	4.77	115.92	110.57
23	BB	306	CHL	C3C-C4C-NC	4.76	115.91	110.57
23	Au	608	CHL	O2D-CGD-CBD	4.75	119.71	111.27
23	BB	302	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
23	r	605	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
23	Au	601	CHL	C3C-C4C-NC	4.74	115.89	110.57
23	Ba	306	CHL	CHB-C1B-NB	-4.74	119.24	124.26
23	r	613	CHL	C3C-C4C-NC	4.74	115.89	110.57
28	BU	616	XAT	C12-C13-C14	-4.74	111.67	118.94
28	Y	301	XAT	C38-C25-C24	-4.73	108.95	114.28
23	0	606	CHL	C3D-C2D-C1D	-4.73	99.37	105.83
23	Y	310	CHL	O2D-CGD-CBD	4.73	119.68	111.27
23	y	307	CHL	CHB-C1B-NB	-4.73	119.25	124.26
23	AB	304	CHL	C3C-C4C-NC	4.73	115.87	110.57
28	BU	616	XAT	O24-C25-C38	-4.72	109.40	115.06
28	N	619	XAT	C8-C9-C10	-4.72	111.70	118.94
23	n	605	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
28	y	301	XAT	C31-C32-C33	-4.72	113.16	126.42
23	BJ	605	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
23	N	608	CHL	C3C-C4C-NC	4.72	115.86	110.57
23	AA	302	CHL	CHB-C1B-NB	-4.72	119.27	124.26
23	Y	302	CHL	C3D-C2D-C1D	-4.71	99.40	105.83
23	y	306	CHL	CHB-C1B-NB	-4.71	119.27	124.26
23	BQ	605	CHL	C3D-C2D-C1D	-4.71	99.40	105.83
28	A2	619	XAT	C8-C9-C10	-4.71	111.71	118.94
23	BU	605	CHL	C3B-C4B-NB	4.70	114.88	110.52
34	BF	517	DGD	O3G-C3G-C2G	-4.70	99.55	110.90
23	g	605	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
23	5	605	CHL	C3C-C4C-NC	4.70	115.84	110.57
23	9	605	CHL	C3C-C4C-NC	4.70	115.84	110.57
23	A6	605	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
28	Ba	301	XAT	C31-C32-C33	-4.70	113.21	126.42
28	Y	301	XAT	O24-C25-C38	-4.70	109.42	115.06
23	A2	608	CHL	C3C-C4C-NC	4.70	115.84	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	604	CLA	C3B-C4B-NB	-4.69	106.16	110.52
23	g	609	CHL	C4A-NA-C1A	4.69	108.81	106.71
34	c	516	DGD	O3G-C3G-C2G	-4.69	99.59	110.90
28	G	619	XAT	C8-C9-C10	-4.69	111.75	118.94
23	S	605	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
23	BV	607	CHL	C3D-C2D-C1D	-4.69	99.44	105.83
28	5	619	XAT	C31-C32-C33	-4.68	113.26	126.42
28	y	301	XAT	O24-C25-C38	-4.68	109.45	115.06
28	Ba	301	XAT	O4-C5-C18	-4.68	109.45	115.06
23	AB	307	CHL	CHB-C1B-NB	-4.67	119.31	124.26
25	9	616	LUT	C15-C35-C34	4.67	133.05	123.47
23	6	606	CHL	C3D-C2D-C1D	-4.67	99.45	105.83
23	BJ	609	CHL	O2D-CGD-CBD	4.67	119.57	111.27
23	A2	607	CHL	C3D-C2D-C1D	-4.67	99.45	105.83
23	r	606	CHL	C3C-C4C-NC	4.67	115.81	110.57
23	6	608	CHL	O2D-CGD-CBD	4.67	119.57	111.27
28	g	619	XAT	C28-C29-C30	-4.67	111.78	118.94
23	BJ	601	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
23	A6	606	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
28	BJ	619	XAT	C28-C29-C30	-4.67	111.78	118.94
23	G	605	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
23	r	605	CHL	C1C-C2C-C3C	-4.67	103.41	107.11
23	BB	309	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
28	Au	619	XAT	O4-C5-C18	-4.66	109.47	115.06
24	5	604	CLA	C3B-C4B-NB	-4.66	106.19	110.52
23	BU	606	CHL	C3C-C4C-NC	4.66	115.80	110.57
23	0	607	CHL	C3C-C4C-NC	4.66	115.80	110.57
23	n	609	CHL	C3C-C4C-NC	4.66	115.80	110.57
23	0	601	CHL	O2D-CGD-CBD	4.66	119.54	111.27
28	7	318	XAT	O24-C25-C38	-4.65	109.48	115.06
23	g	601	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
23	n	606	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
23	6	605	CHL	C3C-C4C-NC	4.65	115.78	110.57
23	g	609	CHL	O2D-CGD-CBD	4.65	119.53	111.27
23	N	607	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
23	S	606	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
28	Au	619	XAT	C8-C9-C10	-4.65	111.81	118.94
23	BU	605	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
23	5	608	CHL	C3C-C4C-NC	4.65	115.78	110.57
28	Y	301	XAT	C8-C9-C10	-4.65	111.81	118.94
23	y	307	CHL	C3D-C2D-C1D	-4.64	99.49	105.83
23	8	304	CHL	C3C-C4C-NC	4.64	115.78	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ba	310	CHL	O2D-CGD-CBD	4.64	119.52	111.27
23	7	302	CHL	CHB-C1B-NB	-4.64	119.34	124.26
23	6	601	CHL	O2D-CGD-CBD	4.64	119.51	111.27
23	y	308	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
23	G	608	CHL	O2D-CGD-CBD	4.64	119.51	111.27
23	6	601	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
28	g	619	XAT	C38-C25-C24	-4.64	109.06	114.28
28	y	301	XAT	O4-C5-C18	-4.63	109.50	115.06
28	BJ	619	XAT	C38-C25-C24	-4.63	109.07	114.28
23	9	608	CHL	C3C-C4C-NC	4.63	115.77	110.57
23	BV	606	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
23	0	601	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
23	Au	607	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
23	BQ	609	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
23	BU	613	CHL	O2D-CGD-CBD	4.63	119.49	111.27
23	9	605	CHL	C3D-C2D-C1D	-4.63	99.52	105.83
23	8	307	CHL	C3C-C4C-NC	4.62	115.76	110.57
23	s	606	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
23	AA	309	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
28	r	616	XAT	O24-C25-C38	-4.62	109.52	115.06
23	7	309	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
28	8	312	XAT	C28-C29-C30	-4.62	111.85	118.94
23	g	606	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
23	BB	308	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
28	9	619	XAT	C25-C24-C23	-4.62	103.62	112.75
23	s	607	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
23	BQ	601	CHL	C3D-C2D-C1D	-4.61	99.53	105.83
23	A2	606	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
28	G	619	XAT	O4-C5-C18	-4.61	109.53	115.06
28	AB	312	XAT	C28-C29-C30	-4.61	111.86	118.94
23	5	605	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	A2	607	CHL	O2D-CGD-CBD	4.61	119.46	111.27
23	BQ	606	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	G	609	CHL	C3C-C4C-NC	4.61	115.74	110.57
23	Ba	308	CHL	C3D-C2D-C1D	-4.61	99.55	105.83
23	6	609	CHL	CHC-C4B-NB	-4.61	119.38	124.26
23	Y	308	CHL	C3D-C2D-C1D	-4.61	99.55	105.83
23	BJ	609	CHL	C4A-NA-C1A	4.60	108.78	106.71
28	AA	301	XAT	C38-C25-C24	-4.60	109.10	114.28
25	BJ	616	LUT	C35-C15-C14	4.60	132.90	123.47
23	BJ	606	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
23	8	306	CHL	C3D-C2D-C1D	-4.60	99.56	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	619	XAT	C18-C5-C4	-4.60	109.11	114.28
23	y	306	CHL	C3D-C2D-C1D	-4.60	99.56	105.83
28	9	619	XAT	C18-C5-C4	-4.60	109.11	114.28
23	Y	309	CHL	C3D-C2D-C1D	-4.60	99.56	105.83
23	n	601	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
25	6	616	LUT	C35-C15-C14	4.59	132.88	123.47
28	Ba	301	XAT	O24-C25-C38	-4.59	109.55	115.06
23	Au	605	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
23	0	605	CHL	C3C-C4C-NC	4.59	115.72	110.57
23	7	308	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
28	AA	301	XAT	C35-C15-C14	-4.59	114.07	123.47
23	BU	613	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
24	s	604	CLA	C3B-C4B-NB	-4.59	106.26	110.52
23	n	609	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
28	BB	301	XAT	C8-C9-C10	-4.58	111.91	118.94
23	AA	308	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
23	Ba	302	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
23	n	609	CHL	CHB-C1B-NB	-4.58	119.41	124.26
23	8	305	CHL	CHB-C1B-NB	-4.58	119.41	124.26
23	AB	305	CHL	CHB-C1B-NB	-4.58	119.41	124.26
23	Ba	306	CHL	C3D-C2D-C1D	-4.58	99.59	105.83
23	Ba	307	CHL	C3D-C2D-C1D	-4.58	99.59	105.83
23	Y	308	CHL	O2D-CGD-CBD	4.58	119.40	111.27
23	AB	306	CHL	C3D-C2D-C1D	-4.58	99.59	105.83
23	BB	307	CHL	C2D-C1D-ND	4.57	113.47	110.10
31	2	404	PL9	C7-C3-C4	4.57	120.59	116.88
23	BH	601	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
23	N	606	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
28	BB	301	XAT	O4-C5-C18	-4.57	109.58	115.06
28	7	301	XAT	C35-C15-C14	-4.57	114.11	123.47
23	BB	308	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
23	A2	605	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
23	AB	306	CHL	O2D-CGD-CBD	4.57	119.39	111.27
23	N	605	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
23	Y	308	CHL	CHD-C4C-C3C	-4.57	118.13	124.84
28	AA	318	XAT	O24-C25-C38	-4.57	109.58	115.06
23	g	607	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
23	BQ	608	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
23	G	601	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
23	BV	607	CHL	C3C-C4C-NC	4.56	115.69	110.57
23	BB	308	CHL	O2D-CGD-CBD	4.56	119.38	111.27
23	n	607	CHL	C3D-C2D-C1D	-4.56	99.61	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	608	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
28	8	312	XAT	C11-C12-C13	-4.56	113.61	126.42
23	Y	307	CHL	C2D-C1D-ND	4.56	113.46	110.10
28	BB	301	XAT	C31-C32-C33	-4.56	113.61	126.42
23	y	302	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
23	r	605	CHL	C3B-C4B-NB	4.55	114.74	110.52
23	6	607	CHL	C3C-C4C-NC	4.55	115.67	110.57
23	BQ	609	CHL	CHB-C1B-NB	-4.55	119.44	124.26
23	G	607	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
28	N	619	XAT	C35-C15-C14	-4.55	114.16	123.47
28	Y	301	XAT	C31-C32-C33	-4.55	113.64	126.42
23	BJ	608	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
28	Y	301	XAT	O4-C5-C18	-4.54	109.61	115.06
23	Au	601	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
25	9	615	LUT	C35-C15-C14	4.54	132.78	123.47
23	n	608	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
38	BD	409	PHO	C2B-C1B-NB	-4.54	106.39	109.53
28	N	619	XAT	C28-C29-C30	-4.54	111.97	118.94
23	BJ	607	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
23	y	309	CHL	C3D-C2D-C1D	-4.54	99.64	105.83
23	G	606	CHL	C3D-C2D-C1D	-4.54	99.64	105.83
23	8	306	CHL	O2D-CGD-CBD	4.54	119.33	111.27
28	g	619	XAT	C8-C9-C10	-4.53	111.98	118.94
23	r	613	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
23	s	607	CHL	C3C-C4C-NC	4.53	115.65	110.57
23	Au	609	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
23	e	601	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
23	A2	608	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
28	Y	301	XAT	C35-C15-C14	-4.53	114.20	123.47
28	7	301	XAT	C38-C25-C24	-4.53	109.19	114.28
23	5	606	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
23	N	601	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
23	G	608	CHL	CHB-C1B-NB	-4.52	119.47	124.26
28	n	619	XAT	C31-C32-C33	-4.52	113.72	126.42
23	BQ	607	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
23	g	608	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
34	C	516	DGD	O3G-C3G-C2G	-4.52	100.00	110.90
23	G	605	CHL	CHB-C1B-NB	-4.52	119.47	124.26
28	AA	318	XAT	C38-C25-C24	-4.52	109.20	114.28
28	AB	312	XAT	C11-C12-C13	-4.52	113.73	126.42
23	S	601	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
25	g	616	LUT	C19-C9-C10	-4.51	116.60	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	601	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
28	g	619	XAT	O24-C25-C38	-4.51	109.65	115.06
28	BB	301	XAT	C35-C15-C14	-4.51	114.23	123.47
23	6	605	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
28	5	619	XAT	C12-C13-C14	-4.51	112.03	118.94
23	AB	304	CHL	C3D-C2D-C1D	-4.50	99.68	105.83
23	N	607	CHL	O2D-CGD-CBD	4.50	119.27	111.27
25	0	616	LUT	C35-C15-C14	4.50	132.70	123.47
28	BJ	619	XAT	C8-C9-C10	-4.50	112.03	118.94
23	0	608	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
38	a	409	PHO	C2B-C1B-NB	-4.50	106.42	109.53
23	6	608	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
28	BJ	619	XAT	O24-C25-C38	-4.50	109.67	115.06
38	A	408	PHO	C2B-C1B-NB	-4.50	106.42	109.53
28	Au	619	XAT	C38-C25-C24	-4.50	109.22	114.28
23	Ba	309	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
23	8	305	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
23	Au	608	CHL	C3C-C4C-NC	4.49	115.61	110.57
23	Au	606	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
23	A6	601	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
23	AB	306	CHL	C3C-C4C-NC	4.49	115.61	110.57
25	5	615	LUT	C35-C15-C14	4.49	132.67	123.47
23	S	607	CHL	CHD-C4C-C3C	-4.49	118.24	124.84
23	y	309	CHL	C3C-C4C-NC	4.49	115.60	110.57
25	5	616	LUT	C19-C9-C10	-4.49	116.64	122.92
23	AB	305	CHL	C3D-C2D-C1D	-4.48	99.71	105.83
23	0	606	CHL	CAC-C3C-C4C	4.48	130.63	124.81
34	1	516	DGD	O3G-C3G-C2G	-4.48	100.10	110.90
28	A2	619	XAT	C35-C15-C14	-4.48	114.30	123.47
23	7	310	CHL	C4A-NA-C1A	4.48	108.72	106.71
23	AA	310	CHL	C4A-NA-C1A	4.48	108.72	106.71
28	8	312	XAT	O24-C25-C38	-4.48	109.69	115.06
28	BQ	619	XAT	O4-C5-C18	-4.48	109.69	115.06
23	G	608	CHL	C3C-C4C-NC	4.47	115.59	110.57
28	A2	619	XAT	C28-C29-C30	-4.47	112.08	118.94
23	0	605	CHL	C3D-C2D-C1D	-4.47	99.73	105.83
23	BQ	609	CHL	C3C-C4C-NC	4.47	115.58	110.57
23	8	304	CHL	C3D-C2D-C1D	-4.47	99.73	105.83
28	BQ	619	XAT	C38-C25-C24	-4.47	109.26	114.28
28	BQ	619	XAT	C31-C32-C33	-4.47	113.87	126.42
23	Y	306	CHL	C3D-C2D-C1D	-4.46	99.74	105.83
23	Ba	309	CHL	C3C-C4C-NC	4.46	115.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	R	407	PHO	C2B-C1B-NB	-4.46	106.45	109.53
28	G	619	XAT	C38-C25-C24	-4.46	109.27	114.28
23	6	606	CHL	CAC-C3C-C4C	4.45	130.59	124.81
23	n	606	CHL	CHB-C1B-NB	-4.45	119.54	124.26
28	AB	312	XAT	O24-C25-C38	-4.45	109.72	115.06
23	y	310	CHL	C3D-C2D-C1D	-4.45	99.75	105.83
23	0	607	CHL	O2D-CGD-CBD	4.45	119.18	111.27
23	BH	601	CHL	CHD-C4C-C3C	-4.45	118.30	124.84
23	y	310	CHL	C4A-NA-C1A	4.45	108.71	106.71
25	9	616	LUT	C19-C9-C10	-4.45	116.69	122.92
23	S	605	CHL	CHD-C4C-C3C	-4.45	118.31	124.84
28	5	619	XAT	C25-C24-C23	-4.45	103.95	112.75
28	BQ	619	XAT	O24-C25-C38	-4.45	109.73	115.06
23	BB	306	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
28	Y	301	XAT	C18-C5-C4	-4.44	109.28	114.28
23	7	307	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
28	BB	301	XAT	C18-C5-C4	-4.44	109.28	114.28
26	Au	617	NEX	C39-C29-C30	-4.44	116.70	122.92
28	n	619	XAT	O4-C5-C18	-4.44	109.74	115.06
23	AA	307	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
28	N	619	XAT	C38-C25-C24	-4.44	109.29	114.28
23	7	306	CHL	C3C-C4C-NC	4.44	115.55	110.57
23	e	601	CHL	CHD-C4C-C3C	-4.43	118.32	124.84
23	9	606	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
23	BB	307	CHL	O2D-CGD-CBD	4.43	119.15	111.27
23	6	607	CHL	O2D-CGD-CBD	4.43	119.14	111.27
23	BV	601	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
23	8	306	CHL	C3C-C4C-NC	4.43	115.54	110.57
23	g	605	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
28	AA	301	XAT	C18-C5-C4	-4.42	109.31	114.28
23	BJ	605	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
23	Au	608	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
23	G	608	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
28	BJ	619	XAT	C31-C32-C33	-4.42	114.00	126.42
23	AA	306	CHL	C3C-C4C-NC	4.42	115.53	110.57
23	s	601	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
23	8	307	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
28	n	619	XAT	O24-C25-C38	-4.42	109.77	115.06
23	AA	310	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
23	Au	605	CHL	CHB-C1B-NB	-4.41	119.58	124.26
23	Y	310	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
28	7	301	XAT	C18-C5-C4	-4.41	109.32	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Y	307	CHL	O2D-CGD-CBD	4.41	119.10	111.27
28	n	619	XAT	C38-C25-C24	-4.41	109.32	114.28
23	BB	310	CHL	C3D-C2D-C1D	-4.41	99.82	105.83
23	6	607	CHL	C3D-C2D-C1D	-4.40	99.82	105.83
28	g	619	XAT	C31-C32-C33	-4.40	114.05	126.42
34	1	517	DGD	O3G-C3G-C2G	-4.40	100.28	110.90
26	G	617	NEX	C39-C29-C30	-4.40	116.76	122.92
23	A6	605	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
23	5	609	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
23	6	606	CHL	O2D-CGD-CBD	4.40	119.08	111.27
23	y	310	CHL	O2D-CGD-CBD	4.40	119.08	111.27
23	AB	307	CHL	C3C-C4C-NC	4.40	115.50	110.57
23	r	605	CHL	O2D-CGD-CBD	4.39	119.08	111.27
28	AA	318	XAT	C18-C5-C4	-4.39	109.34	114.28
28	5	619	XAT	C28-C29-C30	-4.39	112.20	118.94
24	c	512	CLA	O2D-CGD-O1D	-4.39	115.25	123.84
34	a	401	DGD	O3G-C3G-C2G	-4.39	100.32	110.90
23	7	310	CHL	C3D-C2D-C1D	-4.39	99.85	105.83
23	A2	609	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
23	7	306	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
34	C	517	DGD	O3G-C3G-C2G	-4.38	100.33	110.90
28	7	318	XAT	C38-C25-C24	-4.38	109.35	114.28
28	7	318	XAT	C18-C5-C4	-4.38	109.36	114.28
23	N	609	CHL	C3D-C2D-C1D	-4.38	99.86	105.83
28	8	312	XAT	C31-C32-C33	-4.37	114.13	126.42
24	8	308	CLA	CMA-C3A-C2A	-4.37	96.19	113.83
28	N	619	XAT	C31-C32-C33	-4.37	114.13	126.42
28	r	616	XAT	O4-C5-C18	-4.37	109.82	115.06
23	Au	608	CHL	CHB-C1B-NB	-4.37	119.63	124.26
27	0	617	LHG	O4-P-O5	4.37	133.82	112.24
28	y	301	XAT	C38-C25-C24	-4.36	109.37	114.28
28	A2	619	XAT	C31-C32-C33	-4.36	114.16	126.42
34	BD	401	DGD	O3G-C3G-C2G	-4.36	100.37	110.90
28	y	301	XAT	C28-C29-C30	-4.36	112.25	118.94
23	n	605	CHL	CHD-C4C-C3C	-4.36	118.43	124.84
27	6	617	LHG	O4-P-O5	4.36	133.79	112.24
28	Ba	301	XAT	C28-C29-C30	-4.36	112.25	118.94
23	Y	310	CHL	CHB-C1B-NB	-4.35	119.65	124.26
28	Ba	301	XAT	C38-C25-C24	-4.35	109.38	114.28
23	AA	306	CHL	C3D-C2D-C1D	-4.35	99.90	105.83
23	AA	308	CHL	O2D-CGD-CBD	4.34	118.99	111.27
23	A2	601	CHL	O2D-CGD-CBD	4.34	118.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BU	616	XAT	O4-C5-C18	-4.34	109.85	115.06
34	BD	413	DGD	O3G-C3G-C2G	-4.34	100.42	110.90
28	AB	312	XAT	C31-C32-C33	-4.34	114.23	126.42
23	Y	309	CHL	CHB-C1B-NB	-4.33	119.67	124.26
23	AB	307	CHL	C3D-C2D-C1D	-4.33	99.92	105.83
34	a	413	DGD	O3G-C3G-C2G	-4.33	100.45	110.90
23	5	608	CHL	C3D-C2D-C1D	-4.33	99.92	105.83
28	N	619	XAT	O4-C5-C18	-4.33	109.87	115.06
23	Ba	310	CHL	C3D-C2D-C1D	-4.33	99.92	105.83
23	A2	606	CHL	O2D-CGD-CBD	4.32	118.95	111.27
26	BJ	617	NEX	C39-C29-C30	-4.32	116.87	122.92
23	0	606	CHL	CHD-C4C-C3C	-4.32	118.49	124.84
23	BQ	607	CHL	O2D-CGD-CBD	4.32	118.94	111.27
24	c	512	CLA	O2D-CGD-CBD	4.31	118.93	111.27
28	n	619	XAT	C28-C29-C30	-4.31	112.32	118.94
23	9	608	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
34	BF	518	DGD	O3G-C3G-C2G	-4.31	100.51	110.90
23	BQ	605	CHL	CHD-C4C-C3C	-4.31	118.51	124.84
27	1	520	LHG	O4-P-O5	4.31	133.53	112.24
23	n	607	CHL	O2D-CGD-CBD	4.31	118.92	111.27
23	7	308	CHL	O2D-CGD-CBD	4.30	118.91	111.27
23	A2	609	CHL	O2D-CGD-CBD	4.30	118.91	111.27
23	N	606	CHL	O2D-CGD-CBD	4.30	118.91	111.27
23	8	305	CHL	O2D-CGD-CBD	4.30	118.91	111.27
25	9	615	LUT	C19-C9-C10	-4.30	116.90	122.92
23	0	607	CHL	C3D-C2D-C1D	-4.30	99.97	105.83
23	AA	308	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
28	G	619	XAT	C35-C15-C14	-4.29	114.68	123.47
27	A2	618	LHG	O4-P-O5	4.29	133.46	112.24
28	BU	616	XAT	C11-C12-C13	-4.29	114.36	126.42
23	N	601	CHL	O2D-CGD-CBD	4.29	118.89	111.27
23	Au	607	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
28	n	619	XAT	C32-C33-C34	-4.29	112.36	118.94
27	BF	520	LHG	O4-P-O5	4.29	133.44	112.24
27	C	520	LHG	O4-P-O5	4.29	133.43	112.24
28	g	619	XAT	C18-C5-C4	-4.29	109.46	114.28
34	c	517	DGD	O3G-C3G-C2G	-4.28	100.56	110.90
25	g	616	LUT	C35-C15-C14	4.28	132.25	123.47
28	A2	619	XAT	O4-C5-C18	-4.28	109.93	115.06
23	9	609	CHL	C3D-C2D-C1D	-4.28	99.99	105.83
25	Au	616	LUT	C19-C9-C10	-4.28	116.93	122.92
27	N	618	LHG	O4-P-O5	4.28	133.41	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	608	CHL	O2D-CGD-CBD	4.28	118.88	111.27
27	9	618	LHG	O4-P-O5	4.28	133.40	112.24
26	g	617	NEX	C39-C29-C30	-4.28	116.93	122.92
28	BQ	619	XAT	C32-C33-C34	-4.28	112.38	118.94
23	5	606	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
28	5	619	XAT	O4-C5-C18	-4.28	109.93	115.06
25	5	615	LUT	C19-C9-C10	-4.27	116.94	122.92
23	G	609	CHL	C3D-C2D-C1D	-4.27	100.00	105.83
23	A2	606	CHL	CHD-C4C-C3C	-4.27	118.56	124.84
28	9	619	XAT	C28-C29-C30	-4.27	112.39	118.94
23	BU	605	CHL	O2D-CGD-CBD	4.27	118.86	111.27
23	Ba	308	CHL	O2D-CGD-CBD	4.27	118.86	111.27
27	BB	319	LHG	O4-P-O5	4.27	133.35	112.24
27	y	319	LHG	O4-P-O5	4.27	133.35	112.24
23	0	606	CHL	O2D-CGD-CBD	4.27	118.85	111.27
26	Y	318	NEX	C39-C29-C30	-4.26	116.95	122.92
27	c	519	LHG	O4-P-O5	4.26	133.32	112.24
28	A2	619	XAT	C38-C25-C24	-4.26	109.48	114.28
25	5	616	LUT	C15-C35-C34	4.26	132.21	123.47
23	Ba	310	CHL	C3C-C4C-NC	4.26	115.35	110.57
27	Ba	319	LHG	O4-P-O5	4.26	133.31	112.24
27	BU	617	LHG	O4-P-O5	4.26	133.31	112.24
23	G	607	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
23	N	608	CHL	O2D-CGD-CBD	4.26	118.84	111.27
23	S	607	CHL	O2D-CGD-CBD	4.26	118.84	111.27
23	BJ	607	CHL	O2D-CGD-CBD	4.26	118.84	111.27
25	AB	311	LUT	C19-C9-C10	-4.26	116.96	122.92
28	BU	616	XAT	C8-C9-C10	-4.26	112.41	118.94
27	5	618	LHG	O4-P-O5	4.25	133.26	112.24
29	K	101	BCR	C33-C5-C6	-4.25	119.75	124.53
27	Y	319	LHG	O4-P-O5	4.25	133.25	112.24
23	BU	605	CHL	CHB-C1B-NB	-4.25	119.76	124.26
23	9	607	CHL	C3D-C2D-C1D	-4.25	100.03	105.83
28	r	616	XAT	C11-C12-C13	-4.25	114.48	126.42
28	9	619	XAT	O4-C5-C18	-4.25	109.97	115.06
23	y	310	CHL	C3C-C4C-NC	4.25	115.33	110.57
26	BB	318	NEX	C39-C29-C30	-4.25	116.97	122.92
23	6	609	CHL	C3D-C2D-C1D	-4.25	100.03	105.83
27	2	405	LHG	O4-P-O5	4.25	133.24	112.24
23	BJ	608	CHL	C3B-C4B-NB	4.24	114.45	110.52
38	a	408	PHO	C2B-C1B-NB	-4.24	106.60	109.53
28	BQ	619	XAT	C28-C29-C30	-4.24	112.43	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BY	201	LHG	O4-P-O5	4.24	133.21	112.24
27	G	618	LHG	O4-P-O5	4.24	133.19	112.24
23	AA	307	CHL	CHB-C1B-NB	-4.24	119.77	124.26
23	BJ	607	CHL	CHD-C4C-C3C	-4.24	118.61	124.84
23	AB	305	CHL	O2D-CGD-CBD	4.24	118.80	111.27
23	BB	310	CHL	CHB-C1B-NB	-4.24	119.77	124.26
26	s	616	NEX	C39-C29-C30	-4.24	116.99	122.92
23	S	605	CHL	C2D-C1D-ND	4.24	113.23	110.10
23	7	308	CHL	CHD-C4C-C3C	-4.24	118.61	124.84
28	AA	318	XAT	C28-C29-C30	-4.23	112.44	118.94
23	N	609	CHL	CHB-C1B-NB	-4.23	119.78	124.26
27	r	618	LHG	O4-P-O5	4.23	133.17	112.24
28	7	318	XAT	C28-C29-C30	-4.23	112.44	118.94
23	9	607	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
26	5	617	NEX	C39-C29-C30	-4.23	117.00	122.92
27	A0	202	LHG	O4-P-O5	4.23	133.16	112.24
24	C	511	CLA	O2D-CGD-O1D	-4.23	115.57	123.84
28	Au	619	XAT	C35-C15-C14	-4.23	114.81	123.47
28	y	301	XAT	C32-C33-C34	-4.23	112.45	118.94
23	N	606	CHL	CHB-C1B-NB	-4.23	119.78	124.26
28	r	616	XAT	C8-C9-C10	-4.23	112.45	118.94
27	w	201	LHG	O4-P-O5	4.23	133.13	112.24
23	6	606	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
27	n	618	LHG	O4-P-O5	4.23	133.13	112.24
27	B	622	LHG	O4-P-O5	4.22	133.13	112.24
23	g	608	CHL	C3B-C4B-NB	4.22	114.43	110.52
28	BQ	619	XAT	C18-C5-C4	-4.22	109.53	114.28
27	Au	618	LHG	O4-P-O5	4.22	133.11	112.24
23	y	302	CHL	CHB-C1B-NB	-4.22	119.79	124.26
23	A6	607	CHL	O2D-CGD-CBD	4.22	118.77	111.27
27	W	201	LHG	O4-P-O5	4.22	133.11	112.24
27	BQ	618	LHG	O4-P-O5	4.22	133.10	112.24
23	9	606	CHL	CHD-C4C-C3C	-4.22	118.64	124.84
23	BB	309	CHL	CHB-C1B-NB	-4.22	119.79	124.26
23	y	308	CHL	O2D-CGD-CBD	4.22	118.76	111.27
23	A2	609	CHL	CHB-C1B-NB	-4.22	119.79	124.26
27	b	623	LHG	O4-P-O5	4.22	133.09	112.24
27	b	624	LHG	O4-P-O5	4.22	133.09	112.24
27	b	622	LHG	O4-P-O5	4.22	133.08	112.24
27	L	102	LHG	O4-P-O5	4.21	133.07	112.24
27	BE	622	LHG	O4-P-O5	4.21	133.06	112.24
23	A6	607	CHL	C3C-C4C-NC	4.21	115.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BE	623	LHG	O4-P-O5	4.21	133.06	112.24
26	BV	616	NEX	C39-C29-C30	-4.21	117.02	122.92
23	A6	601	CHL	CAC-C3C-C4C	4.21	130.27	124.81
26	A2	617	NEX	C39-C29-C30	-4.21	117.03	122.92
28	Ba	301	XAT	C32-C33-C34	-4.21	112.48	118.94
23	g	609	CHL	C3D-C2D-C1D	-4.21	100.09	105.83
23	A2	606	CHL	CHB-C1B-NB	-4.21	119.80	124.26
27	Az	102	LHG	O4-P-O5	4.21	133.04	112.24
23	g	607	CHL	O2D-CGD-CBD	4.21	118.74	111.27
26	BQ	617	NEX	C35-C15-C14	4.21	132.09	123.47
28	BJ	619	XAT	C18-C5-C4	-4.20	109.55	114.28
26	9	617	NEX	C39-C29-C30	-4.20	117.03	122.92
27	BJ	618	LHG	O4-P-O5	4.20	133.02	112.24
23	BQ	609	CHL	O2D-CGD-CBD	4.20	118.73	111.27
23	N	609	CHL	O2D-CGD-CBD	4.20	118.73	111.27
23	N	605	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
38	BD	408	PHO	C2B-C1B-NB	-4.20	106.63	109.53
23	A6	605	CHL	CAC-C3C-C4C	4.20	130.26	124.81
25	G	616	LUT	C19-C9-C10	-4.20	117.04	122.92
27	BE	624	LHG	O4-P-O5	4.20	132.98	112.24
23	A6	605	CHL	C2D-C1D-ND	4.20	113.20	110.10
27	1	521	LHG	O4-P-O5	4.19	132.97	112.24
25	r	615	LUT	C19-C9-C10	-4.19	117.05	122.92
23	s	607	CHL	O2D-CGD-CBD	4.19	118.72	111.27
28	A2	619	XAT	C32-C33-C34	-4.19	112.51	118.94
23	A2	605	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
23	6	609	CHL	O2D-CGD-CBD	4.19	118.71	111.27
27	g	618	LHG	O4-P-O5	4.19	132.94	112.24
27	C	521	LHG	O4-P-O5	4.19	132.93	112.24
28	BJ	619	XAT	O4-C5-C18	-4.18	110.04	115.06
27	B	621	LHG	O4-P-O5	4.18	132.92	112.24
26	BB	320	NEX	C39-C29-C30	-4.18	117.06	122.92
23	BJ	601	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
25	BU	615	LUT	C19-C9-C10	-4.18	117.07	122.92
23	Y	308	CHL	C3B-C4B-NB	4.18	114.39	110.52
28	Au	619	XAT	C28-C29-C30	-4.18	112.53	118.94
23	n	609	CHL	O2D-CGD-CBD	4.17	118.69	111.27
23	N	606	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
23	BJ	609	CHL	C3D-C2D-C1D	-4.17	100.14	105.83
28	g	619	XAT	O4-C5-C18	-4.17	110.06	115.06
23	9	601	CHL	O2D-CGD-CBD	4.17	118.68	111.27
23	A2	607	CHL	CHD-C4C-C3C	-4.17	118.71	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	r	605	CHL	CHB-C1B-NB	-4.17	119.84	124.26
28	G	619	XAT	C32-C33-C34	-4.17	112.54	118.94
26	N	617	NEX	C39-C29-C30	-4.17	117.08	122.92
28	5	619	XAT	C8-C9-C10	-4.17	112.54	118.94
23	g	605	CHL	C2D-C1D-ND	4.17	113.18	110.10
26	A6	616	NEX	C39-C29-C30	-4.17	117.08	122.92
26	r	617	NEX	C39-C29-C30	-4.17	117.09	122.92
27	v	621	LHG	O4-P-O5	4.17	132.84	112.24
23	g	601	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
28	n	619	XAT	C18-C5-C4	-4.16	109.59	114.28
26	S	616	NEX	C39-C29-C30	-4.16	117.09	122.92
23	BV	606	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
23	s	606	CHL	C2D-C1D-ND	4.16	113.17	110.10
23	s	606	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
23	Au	601	CHL	CAC-C3C-C4C	4.16	130.21	124.81
27	BF	521	LHG	O4-P-O5	4.16	132.78	112.24
23	BJ	605	CHL	C2D-C1D-ND	4.16	113.17	110.10
25	6	616	LUT	C39-C29-C30	-4.15	117.11	122.92
23	y	307	CHL	O2D-CGD-CBD	4.15	118.65	111.27
31	D	403	PL9	C7-C3-C4	4.15	120.25	116.88
26	y	318	NEX	C39-C29-C30	-4.15	117.11	122.92
28	G	619	XAT	C28-C29-C30	-4.15	112.57	118.94
23	0	605	CHL	O2D-CGD-CBD	4.15	118.64	111.27
28	AB	312	XAT	C38-C25-C24	-4.15	109.61	114.28
23	9	608	CHL	O2D-CGD-CBD	4.15	118.64	111.27
23	Ba	307	CHL	O2D-CGD-CBD	4.15	118.64	111.27
23	BJ	609	CHL	C3C-C4C-NC	4.15	115.22	110.57
23	Ba	302	CHL	CHB-C1B-NB	-4.15	119.87	124.26
23	A6	607	CHL	C4A-NA-C1A	4.15	108.57	106.71
24	AB	308	CLA	CMA-C3A-C2A	-4.15	97.11	113.83
23	BB	308	CHL	C3B-C4B-NB	4.14	114.36	110.52
27	d	404	LHG	O4-P-O5	4.14	132.72	112.24
27	2	406	LHG	O4-P-O5	4.14	132.72	112.24
28	AA	301	XAT	C8-C9-C10	-4.14	112.58	118.94
28	7	301	XAT	C8-C9-C10	-4.14	112.58	118.94
25	N	616	LUT	C39-C29-C30	-4.14	117.12	122.92
28	7	318	XAT	O4-C5-C18	-4.14	110.09	115.06
27	c	520	LHG	O4-P-O5	4.14	132.71	112.24
23	BQ	607	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
25	A2	616	LUT	C39-C29-C30	-4.14	117.12	122.92
23	BV	606	CHL	C2D-C1D-ND	4.14	113.16	110.10
23	S	605	CHL	CAC-C3C-C4C	4.14	130.18	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Au	619	XAT	C32-C33-C34	-4.14	112.59	118.94
27	D	404	LHG	O4-P-O5	4.14	132.69	112.24
23	BB	308	CHL	C2D-C1D-ND	4.13	113.15	110.10
27	BG	404	LHG	O4-P-O5	4.13	132.67	112.24
23	0	609	CHL	C3D-C2D-C1D	-4.13	100.20	105.83
23	G	607	CHL	O2D-CGD-CBD	4.13	118.61	111.27
23	0	601	CHL	CAC-C3C-C4C	4.13	130.17	124.81
26	7	319	NEX	C35-C15-C14	4.13	131.93	123.47
25	5	615	LUT	C39-C29-C30	-4.13	117.14	122.92
23	G	606	CHL	O2D-CGD-CBD	4.13	118.60	111.27
23	g	609	CHL	C3C-C4C-NC	4.13	115.20	110.57
23	G	605	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
23	g	607	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
23	y	309	CHL	C4A-NA-C1A	4.13	108.56	106.71
23	Au	606	CHL	O2D-CGD-CBD	4.12	118.60	111.27
28	AB	312	XAT	C20-C13-C12	-4.12	111.58	118.08
26	BJ	617	NEX	C35-C15-C14	4.12	131.92	123.47
25	A2	616	LUT	C19-C9-C10	-4.12	117.15	122.92
23	BV	607	CHL	O2D-CGD-CBD	4.12	118.59	111.27
25	9	615	LUT	C39-C29-C30	-4.12	117.15	122.92
23	Y	309	CHL	C1-C2-C3	-4.12	118.91	126.04
28	N	619	XAT	C32-C33-C34	-4.12	112.62	118.94
28	r	616	XAT	C28-C29-C30	-4.12	112.62	118.94
23	g	601	CHL	C2D-C1D-ND	4.12	113.14	110.10
23	BB	309	CHL	C1-C2-C3	-4.12	118.92	126.04
25	BB	317	LUT	C19-C9-C10	-4.12	117.16	122.92
28	AA	318	XAT	O4-C5-C18	-4.12	110.12	115.06
34	A	402	DGD	O3G-C3G-C2G	-4.12	100.97	110.90
23	A2	601	CHL	CHD-C4C-C3C	-4.11	118.79	124.84
23	S	601	CHL	CAC-C3C-C4C	4.11	130.15	124.81
28	8	312	XAT	C8-C9-C10	-4.11	112.63	118.94
26	AA	319	NEX	C35-C15-C14	4.11	131.90	123.47
23	n	606	CHL	O2D-CGD-CBD	4.11	118.58	111.27
23	6	605	CHL	O2D-CGD-CBD	4.11	118.58	111.27
23	N	601	CHL	CHD-C4C-C3C	-4.11	118.80	124.84
25	AA	316	LUT	C19-C9-C10	-4.11	117.17	122.92
23	5	607	CHL	C3D-C2D-C1D	-4.11	100.22	105.83
23	Au	607	CHL	O2D-CGD-CBD	4.11	118.56	111.27
23	BJ	601	CHL	C2D-C1D-ND	4.10	113.13	110.10
23	BQ	601	CHL	CHB-C1B-NB	-4.10	119.91	124.26
26	Ba	318	NEX	C39-C29-C30	-4.10	117.17	122.92
26	BQ	617	NEX	C39-C29-C30	-4.10	117.18	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BH	601	CHL	C2D-C1D-ND	4.10	113.13	110.10
25	Au	615	LUT	C19-C9-C10	-4.10	117.18	122.92
28	8	312	XAT	C20-C13-C12	-4.10	111.62	118.08
23	n	607	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
23	0	609	CHL	CHC-C4B-NB	-4.10	119.92	124.26
26	7	319	NEX	C39-C29-C30	-4.10	117.18	122.92
23	N	607	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
28	8	312	XAT	C38-C25-C24	-4.09	109.67	114.28
23	n	601	CHL	CHB-C1B-NB	-4.09	119.92	124.26
23	5	601	CHL	O2D-CGD-CBD	4.09	118.54	111.27
25	Y	317	LUT	C19-C9-C10	-4.09	117.19	122.92
34	R	401	DGD	O3G-C3G-C2G	-4.09	101.02	110.90
28	7	301	XAT	C28-C29-C30	-4.09	112.66	118.94
23	BQ	606	CHL	O2D-CGD-CBD	4.09	118.54	111.27
23	y	309	CHL	C1-C2-C3	-4.09	118.97	126.04
23	Au	606	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
24	5	604	CLA	CHB-C1B-NB	4.09	128.59	124.26
23	6	601	CHL	CAC-C3C-C4C	4.09	130.11	124.81
23	s	601	CHL	CHB-C1B-NB	-4.08	119.93	124.26
26	n	617	NEX	C39-C29-C30	-4.08	117.20	122.92
25	y	317	LUT	C39-C29-C30	-4.08	117.20	122.92
23	7	307	CHL	CHB-C1B-NB	-4.08	119.94	124.26
23	BU	607	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
23	S	607	CHL	C2D-C1D-ND	4.08	113.11	110.10
25	7	316	LUT	C39-C29-C30	-4.08	117.21	122.92
23	N	605	CHL	CHB-C1B-NB	-4.08	119.94	124.26
25	N	615	LUT	C15-C35-C34	4.08	131.83	123.47
25	N	616	LUT	C19-C9-C10	-4.08	117.21	122.92
23	G	605	CHL	C2D-C1D-ND	4.07	113.11	110.10
23	0	606	CHL	C2D-C1D-ND	4.07	113.11	110.10
23	s	607	CHL	CAC-C3C-C4C	4.07	130.09	124.81
23	n	601	CHL	O2D-CGD-CBD	4.07	118.51	111.27
25	G	615	LUT	C19-C9-C10	-4.07	117.22	122.92
24	9	604	CLA	CHB-C1B-NB	4.07	128.57	124.26
28	AA	301	XAT	O4-C5-C18	-4.07	110.18	115.06
23	BU	607	CHL	CAC-C3C-C4C	4.07	130.09	124.81
25	AB	311	LUT	C15-C35-C34	4.07	131.81	123.47
25	6	616	LUT	C19-C9-C10	-4.06	117.23	122.92
23	BQ	601	CHL	O2D-CGD-CBD	4.06	118.49	111.27
23	BB	309	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
23	Ba	309	CHL	C1-C2-C3	-4.06	119.02	126.04
23	BQ	605	CHL	C2D-C1D-ND	4.06	113.10	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ba	308	CHL	CHD-C4C-C3C	-4.06	118.88	124.84
23	5	601	CHL	C2D-C1D-ND	4.06	113.09	110.10
25	0	616	LUT	C39-C29-C30	-4.06	117.24	122.92
25	0	616	LUT	C19-C9-C10	-4.05	117.24	122.92
25	Ba	317	LUT	C39-C29-C30	-4.05	117.24	122.92
28	7	301	XAT	O4-C5-C18	-4.05	110.20	115.06
23	r	607	CHL	C3B-C4B-NB	4.05	114.28	110.52
23	BU	607	CHL	C3B-C4B-NB	4.05	114.28	110.52
23	5	608	CHL	O2D-CGD-CBD	4.05	118.47	111.27
23	BJ	605	CHL	O2D-CGD-CBD	4.05	118.47	111.27
24	AB	310	CLA	CAA-C2A-C3A	-4.05	101.68	112.78
23	G	606	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
23	y	302	CHL	C6-C5-C3	-4.05	108.00	114.62
28	AA	318	XAT	C8-C9-C10	-4.05	112.73	118.94
32	2	408	SQD	O47-C7-C8	4.05	120.22	111.50
23	e	601	CHL	C2D-C1D-ND	4.05	113.09	110.10
28	7	318	XAT	C8-C9-C10	-4.04	112.73	118.94
32	BD	412	SQD	O47-C7-C8	4.04	120.22	111.50
25	AA	316	LUT	C35-C15-C14	4.04	131.76	123.47
23	Au	609	CHL	C3B-C4B-NB	4.04	114.27	110.52
28	9	619	XAT	C19-C9-C8	-4.04	111.71	118.08
23	y	308	CHL	CHD-C4C-C3C	-4.04	118.90	124.84
26	g	617	NEX	C35-C15-C14	4.04	131.75	123.47
23	n	605	CHL	C2D-C1D-ND	4.04	113.08	110.10
28	N	619	XAT	C18-C5-C4	-4.04	109.74	114.28
23	Ba	309	CHL	C4A-NA-C1A	4.04	108.52	106.71
23	BJ	608	CHL	CAC-C3C-C4C	4.04	130.05	124.81
23	g	606	CHL	CHD-C4C-C3C	-4.04	118.91	124.84
28	A2	619	XAT	C18-C5-C4	-4.04	109.74	114.28
23	7	308	CHL	C2D-C1D-ND	4.04	113.08	110.10
28	Au	619	XAT	C31-C32-C33	-4.04	115.08	126.42
28	BU	616	XAT	C28-C29-C30	-4.03	112.75	118.94
23	g	605	CHL	O2D-CGD-CBD	4.03	118.44	111.27
23	n	606	CHL	CHD-C4C-C3C	-4.03	118.91	124.84
23	s	605	CHL	C3D-C2D-C1D	-4.03	100.33	105.83
26	AA	319	NEX	C39-C29-C30	-4.03	117.27	122.92
28	g	619	XAT	C32-C33-C34	-4.03	112.75	118.94
23	0	609	CHL	CAC-C3C-C4C	4.03	130.04	124.81
23	AA	308	CHL	C2D-C1D-ND	4.03	113.08	110.10
23	9	601	CHL	C2D-C1D-ND	4.03	113.07	110.10
28	G	619	XAT	C31-C32-C33	-4.03	115.09	126.42
23	BV	607	CHL	CAC-C3C-C4C	4.03	130.04	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	607	CHL	CHB-C1B-NB	-4.03	119.99	124.26
23	Au	609	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
23	r	607	CHL	C2D-C1D-ND	4.03	113.07	110.10
23	BJ	601	CHL	C3B-C4B-NB	4.03	114.25	110.52
28	AA	301	XAT	C28-C29-C30	-4.03	112.76	118.94
28	BU	616	XAT	C30-C31-C32	-4.03	110.65	123.22
23	A2	605	CHL	CMB-C2B-C1B	4.02	131.50	125.37
32	a	412	SQD	O7-S-C6	4.02	111.72	106.94
23	6	606	CHL	C2D-C1D-ND	4.02	113.07	110.10
26	9	617	NEX	C15-C35-C34	4.02	131.71	123.47
23	Ba	307	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
25	AA	316	LUT	C39-C29-C30	-4.02	117.29	122.92
38	R	408	PHO	C2B-C1B-NB	-4.02	106.75	109.53
32	BG	406	SQD	O47-C7-C8	4.02	120.16	111.50
25	Ba	317	LUT	C19-C9-C10	-4.02	117.29	122.92
38	A	409	PHO	C2B-C1B-NB	-4.02	106.75	109.53
23	0	606	CHL	C3B-C4B-NB	4.02	114.24	110.52
23	6	607	CHL	CAC-C3C-C4C	4.01	130.02	124.81
23	Ba	307	CHL	CAC-C3C-C4C	4.01	130.02	124.81
23	BJ	606	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
23	BB	302	CHL	CAC-C3C-C4C	4.01	130.01	124.81
26	5	617	NEX	C15-C35-C34	4.01	131.69	123.47
23	Y	309	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
24	8	310	CLA	CAA-C2A-C3A	-4.01	101.80	112.78
32	l	101	SQD	O47-C7-C8	4.01	120.14	111.50
23	A2	605	CHL	CHB-C1B-NB	-4.01	120.02	124.26
28	AB	312	XAT	C10-C11-C12	-4.00	110.72	123.22
25	g	615	LUT	C19-C9-C10	-4.00	117.31	122.92
26	7	319	NEX	C15-C35-C34	4.00	131.68	123.47
26	AA	319	NEX	C15-C35-C34	4.00	131.68	123.47
23	Y	308	CHL	C2D-C1D-ND	4.00	113.06	110.10
23	AB	304	CHL	O2D-CGD-CBD	4.00	118.38	111.27
23	g	606	CHL	O2D-CGD-CBD	4.00	118.38	111.27
28	BJ	619	XAT	C32-C33-C34	-4.00	112.80	118.94
23	r	607	CHL	CAC-C3C-C4C	4.00	130.00	124.81
25	BB	316	LUT	C19-C9-C10	-4.00	117.32	122.92
25	n	616	LUT	C19-C9-C10	-4.00	117.32	122.92
28	5	619	XAT	C20-C13-C12	-4.00	111.77	118.08
23	r	607	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
23	g	601	CHL	C3B-C4B-NB	4.00	114.23	110.52
32	BO	101	SQD	O47-C7-C8	4.00	120.12	111.50
23	7	309	CHL	O2D-CGD-CBD	4.00	118.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	606	CHL	C3B-C4B-NB	4.00	114.22	110.52
32	d	406	SQD	O47-C7-C8	4.00	120.11	111.50
23	BJ	609	CHL	CHC-C4B-NB	-4.00	120.03	124.26
25	y	317	LUT	C19-C9-C10	-4.00	117.33	122.92
23	AA	309	CHL	O2D-CGD-CBD	3.99	118.37	111.27
34	C	518	DGD	O3G-C3G-C2G	-3.99	101.26	110.90
23	A2	607	CHL	C2D-C1D-ND	3.99	113.05	110.10
28	r	616	XAT	C30-C31-C32	-3.99	110.75	123.22
25	Y	316	LUT	C19-C9-C10	-3.99	117.33	122.92
23	BV	601	CHL	CHB-C1B-NB	-3.99	120.03	124.26
32	D	406	SQD	O9-S-C6	3.99	111.68	106.94
23	g	608	CHL	CAC-C3C-C4C	3.99	129.99	124.81
23	Au	607	CHL	C2D-C1D-ND	3.99	113.05	110.10
23	N	601	CHL	C3B-C4B-NB	3.99	114.22	110.52
26	BB	318	NEX	C35-C15-C14	3.99	131.65	123.47
23	BJ	606	CHL	O2D-CGD-CBD	3.99	118.36	111.27
23	A2	601	CHL	C3B-C4B-NB	3.99	114.21	110.52
28	G	619	XAT	C18-C5-C4	-3.99	109.80	114.28
32	BD	412	SQD	O7-S-C6	3.99	111.68	106.94
23	y	307	CHL	CHD-C4C-C3C	-3.98	118.99	124.84
23	A2	605	CHL	C3B-C4B-NB	3.98	114.21	110.52
23	9	608	CHL	CAC-C3C-C4C	3.98	129.97	124.81
23	g	609	CHL	CHC-C4B-NB	-3.98	120.05	124.26
23	BQ	606	CHL	CAC-C3C-C4C	3.97	129.97	124.81
28	7	318	XAT	C12-C13-C14	-3.97	112.84	118.94
28	8	312	XAT	C10-C11-C12	-3.97	110.82	123.22
23	5	608	CHL	CAC-C3C-C4C	3.97	129.96	124.81
23	N	605	CHL	C3B-C4B-NB	3.97	114.20	110.52
32	a	412	SQD	O47-C7-C8	3.97	120.06	111.50
25	7	316	LUT	C19-C9-C10	-3.97	117.36	122.92
28	9	619	XAT	C32-C33-C34	-3.97	112.85	118.94
25	BQ	616	LUT	C19-C9-C10	-3.97	117.36	122.92
23	6	607	CHL	CHB-C1B-NB	-3.97	120.06	124.26
25	Y	317	LUT	C39-C29-C30	-3.97	117.36	122.92
28	9	619	XAT	C8-C9-C10	-3.97	112.86	118.94
23	N	607	CHL	C2D-C1D-ND	3.97	113.03	110.10
23	7	307	CHL	O2D-CGD-CBD	3.96	118.31	111.27
28	BU	616	XAT	C32-C33-C34	-3.96	112.86	118.94
26	Au	617	NEX	C15-C35-C34	3.96	131.59	123.47
23	BB	302	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
28	7	301	XAT	C31-C32-C33	-3.96	115.29	126.42
23	0	607	CHL	CAC-C3C-C4C	3.96	129.95	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	318	NEX	C35-C15-C14	3.96	131.58	123.47
23	Y	302	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
25	A6	615	LUT	C19-C9-C10	-3.96	117.38	122.92
23	y	307	CHL	CAC-C3C-C4C	3.95	129.94	124.81
25	BJ	615	LUT	C19-C9-C10	-3.95	117.39	122.92
23	AA	307	CHL	O2D-CGD-CBD	3.95	118.29	111.27
23	g	608	CHL	C2D-C1D-ND	3.95	113.02	110.10
23	n	606	CHL	CAC-C3C-C4C	3.95	129.94	124.81
25	n	616	LUT	C39-C29-C30	-3.95	117.39	122.92
28	Ba	301	XAT	C18-C5-C4	-3.95	109.84	114.28
28	Au	619	XAT	C18-C5-C4	-3.95	109.84	114.28
28	BU	616	XAT	C31-C32-C33	-3.95	115.33	126.42
26	G	617	NEX	C15-C35-C34	3.94	131.55	123.47
23	g	605	CHL	C3B-C4B-NB	3.94	114.17	110.52
25	AA	317	LUT	C19-C9-C10	-3.94	117.40	122.92
23	8	304	CHL	O2D-CGD-CBD	3.94	118.27	111.27
28	AA	301	XAT	C31-C32-C33	-3.94	115.35	126.42
23	AA	310	CHL	C3C-C4C-NC	3.94	114.99	110.57
23	0	609	CHL	O2D-CGD-CBD	3.94	118.27	111.27
23	Y	302	CHL	CAC-C3C-C4C	3.93	129.91	124.81
28	AA	318	XAT	C12-C13-C14	-3.93	112.91	118.94
23	Au	601	CHL	C3B-C4B-NB	3.93	114.16	110.52
26	A2	617	NEX	C12-C13-C14	3.93	124.97	118.94
23	BV	605	CHL	C3D-C2D-C1D	-3.93	100.47	105.83
25	7	317	LUT	C19-C9-C10	-3.93	117.42	122.92
23	G	601	CHL	CHD-C4C-C3C	-3.93	119.07	124.84
25	A2	615	LUT	C15-C35-C34	3.93	131.52	123.47
25	9	616	LUT	C39-C29-C30	-3.92	117.43	122.92
32	L	101	SQD	O9-S-C6	3.92	111.59	106.94
25	BQ	616	LUT	C39-C29-C30	-3.91	117.44	122.92
23	7	310	CHL	C3C-C4C-NC	3.91	114.96	110.57
23	y	308	CHL	C2D-C1D-ND	3.91	112.99	110.10
25	BB	317	LUT	C39-C29-C30	-3.91	117.44	122.92
28	5	619	XAT	C19-C9-C8	-3.91	111.92	118.08
26	N	617	NEX	C35-C15-C14	3.91	131.48	123.47
34	1	518	DGD	O3G-C3G-C2G	-3.91	101.47	110.90
23	N	605	CHL	CMB-C2B-C1B	3.91	131.32	125.37
32	2	408	SQD	O9-S-C6	3.91	111.58	106.94
24	b	611	CLA	CAC-C3C-C2C	3.91	134.21	127.53
25	7	317	LUT	C39-C29-C30	-3.91	117.45	122.92
32	A1	101	SQD	O47-C7-C8	3.91	119.92	111.50
23	S	606	CHL	CHD-C4C-C3C	-3.91	119.10	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	616	XAT	C31-C32-C33	-3.90	115.45	126.42
26	A6	616	NEX	C35-C15-C14	3.90	131.47	123.47
23	r	605	CHL	C2D-C1D-ND	3.90	112.98	110.10
23	BU	607	CHL	C2D-C1D-ND	3.90	112.98	110.10
23	BJ	608	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
28	9	619	XAT	C10-C11-C12	-3.90	111.06	123.22
23	BJ	608	CHL	C2D-C1D-ND	3.90	112.97	110.10
23	A6	606	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
24	6	604	CLA	CAC-C3C-C4C	-3.89	119.76	124.81
25	Au	616	LUT	C39-C29-C30	-3.89	117.47	122.92
25	Ba	316	LUT	C19-C9-C10	-3.89	117.47	122.92
26	A2	617	NEX	C17-C1-C6	3.89	113.95	110.47
25	5	616	LUT	C39-C29-C30	-3.89	117.48	122.92
25	G	616	LUT	C39-C29-C30	-3.89	117.48	122.92
23	BJ	605	CHL	C3B-C4B-NB	3.88	114.12	110.52
23	N	609	CHL	CHD-C4C-C3C	-3.88	119.13	124.84
23	S	605	CHL	C1D-ND-C4D	-3.88	103.58	106.33
23	Y	307	CHL	CAC-C3C-C4C	3.88	129.84	124.81
26	g	617	NEX	C15-C35-C34	3.88	131.42	123.47
29	BN	101	BCR	C33-C5-C6	-3.88	120.17	124.53
32	D	406	SQD	O47-C7-C8	3.88	119.86	111.50
28	AB	312	XAT	C8-C9-C10	-3.88	112.99	118.94
23	A2	605	CHL	O2D-CGD-CBD	3.88	118.16	111.27
26	y	318	NEX	C35-C15-C14	3.87	131.40	123.47
23	A2	609	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
25	8	311	LUT	C19-C9-C10	-3.87	117.50	122.92
34	h	102	DGD	O3G-C3G-C2G	-3.87	101.57	110.90
23	G	601	CHL	C3B-C4B-NB	3.86	114.10	110.52
25	n	616	LUT	C35-C15-C14	3.86	131.39	123.47
25	s	615	LUT	C39-C29-C30	-3.86	117.51	122.92
32	R	411	SQD	O47-C7-C8	3.86	119.83	111.50
32	L	103	SQD	O47-C7-C8	3.86	119.83	111.50
23	AA	306	CHL	O2D-CGD-CBD	3.86	118.13	111.27
23	AB	307	CHL	O2D-CGD-CBD	3.86	118.13	111.27
23	0	607	CHL	C3B-C4B-NB	3.86	114.10	110.52
24	G	611	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
23	0	608	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
23	7	306	CHL	O2D-CGD-CBD	3.85	118.11	111.27
25	S	615	LUT	C19-C9-C10	-3.85	117.53	122.92
26	s	616	NEX	C35-C15-C14	3.85	131.36	123.47
25	y	316	LUT	C39-C29-C30	-3.85	117.53	122.92
23	Au	605	CHL	C2D-C1D-ND	3.85	112.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BV	616	NEX	C35-C15-C14	3.85	131.35	123.47
25	BV	615	LUT	C19-C9-C10	-3.85	117.53	122.92
26	Ba	318	NEX	C35-C15-C14	3.85	131.35	123.47
25	N	616	LUT	C35-C15-C14	3.84	131.35	123.47
23	BJ	607	CHL	C2D-C1D-ND	3.84	112.94	110.10
23	9	607	CHL	C3B-C4B-NB	3.84	114.08	110.52
23	S	601	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
25	BV	615	LUT	C39-C29-C30	-3.84	117.54	122.92
28	y	301	XAT	C18-C5-C4	-3.84	109.96	114.28
25	y	316	LUT	C19-C9-C10	-3.84	117.54	122.92
23	g	605	CHL	C1D-ND-C4D	-3.84	103.61	106.33
23	n	605	CHL	O2D-CGD-CBD	3.84	118.09	111.27
25	s	615	LUT	C19-C9-C10	-3.84	117.55	122.92
23	g	608	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
26	BQ	617	NEX	C15-C35-C34	3.84	131.33	123.47
28	5	619	XAT	C30-C31-C32	-3.83	111.25	123.22
32	A1	101	SQD	O7-S-C6	3.83	111.50	106.94
26	9	617	NEX	C35-C15-C14	3.83	131.33	123.47
25	AA	317	LUT	C39-C29-C30	-3.83	117.55	122.92
25	8	311	LUT	C39-C29-C30	-3.83	117.56	122.92
23	BB	302	CHL	C2D-C1D-ND	3.83	112.93	110.10
23	G	608	CHL	CAC-C3C-C4C	3.83	129.78	124.81
23	7	307	CHL	CHD-C4C-C3C	-3.83	119.21	124.84
26	5	617	NEX	C35-C15-C14	3.83	131.32	123.47
23	g	601	CHL	C1D-ND-C4D	-3.83	103.61	106.33
25	0	615	LUT	C19-C9-C10	-3.83	117.56	122.92
23	s	605	CHL	CAC-C3C-C4C	3.83	129.77	124.81
23	N	605	CHL	O2D-CGD-CBD	3.83	118.07	111.27
23	Au	607	CHL	CAC-C3C-C4C	3.82	129.77	124.81
25	Ba	316	LUT	C39-C29-C30	-3.82	117.57	122.92
26	BJ	617	NEX	C15-C35-C34	3.82	131.31	123.47
23	BJ	605	CHL	C1D-ND-C4D	-3.82	103.62	106.33
25	BQ	615	LUT	C39-C29-C30	-3.82	117.57	122.92
25	A2	616	LUT	C35-C15-C14	3.82	131.30	123.47
23	BQ	608	CHL	O2D-CGD-CBD	3.82	118.06	111.27
23	s	606	CHL	C3B-C4B-NB	3.82	114.06	110.52
32	BO	102	SQD	O9-S-O7	-3.82	100.73	113.95
23	A2	607	CHL	CAC-C3C-C4C	3.82	129.76	124.81
25	Au	616	LUT	C35-C15-C14	3.82	131.29	123.47
28	r	616	XAT	C38-C25-C24	-3.82	109.98	114.28
26	r	617	NEX	C35-C15-C14	3.82	131.29	123.47
23	7	309	CHL	CAC-C3C-C4C	3.82	129.76	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	616	LUT	C39-C29-C30	-3.81	117.58	122.92
25	n	615	LUT	C39-C29-C30	-3.81	117.58	122.92
23	n	608	CHL	O2D-CGD-CBD	3.81	118.05	111.27
23	7	309	CHL	C3B-C4B-NB	3.81	114.05	110.52
23	BB	310	CHL	CAC-C3C-C4C	3.81	129.76	124.81
23	BQ	605	CHL	O2D-CGD-CBD	3.81	118.04	111.27
26	A2	617	NEX	C35-C15-C14	3.81	131.28	123.47
23	BV	605	CHL	CAC-C3C-C4C	3.81	129.76	124.81
23	A6	606	CHL	C2D-C1D-ND	3.81	112.91	110.10
26	S	616	NEX	C35-C15-C14	3.81	131.28	123.47
23	A2	607	CHL	C3B-C4B-NB	3.81	114.05	110.52
26	n	617	NEX	C35-C15-C14	3.81	131.28	123.47
23	n	607	CHL	CHB-C1B-NB	-3.81	120.22	124.26
31	d	403	PL9	C27-C26-C24	-3.81	100.45	112.98
23	Y	310	CHL	CAC-C3C-C4C	3.81	129.75	124.81
23	5	607	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
23	A6	601	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
25	BB	316	LUT	C15-C35-C34	3.81	131.27	123.47
23	Ba	308	CHL	C2D-C1D-ND	3.81	112.91	110.10
23	BU	606	CHL	O2D-CGD-CBD	3.80	118.03	111.27
23	g	607	CHL	C2D-C1D-ND	3.80	112.91	110.10
32	l	102	SQD	O9-S-O7	-3.80	100.79	113.95
23	9	609	CHL	CHC-C4B-NB	-3.80	120.23	124.26
32	d	406	SQD	O9-S-C6	3.80	111.46	106.94
23	A6	601	CHL	CHB-C1B-NB	-3.80	120.23	124.26
23	BB	302	CHL	C1-C2-C3	-3.80	119.47	126.04
23	AA	307	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
28	r	616	XAT	C19-C9-C8	-3.80	112.10	118.08
23	BQ	606	CHL	CHD-C4C-C3C	-3.79	119.26	124.84
26	n	617	NEX	C15-C35-C34	3.79	131.25	123.47
23	Au	608	CHL	CAC-C3C-C4C	3.79	129.73	124.81
23	Y	302	CHL	C2D-C1D-ND	3.79	112.90	110.10
32	D	406	SQD	O9-S-O7	-3.79	100.83	113.95
23	BB	307	CHL	CAC-C3C-C4C	3.79	129.73	124.81
23	5	605	CHL	O2D-CGD-CBD	3.79	118.00	111.27
23	S	606	CHL	C2D-C1D-ND	3.79	112.90	110.10
32	A	413	SQD	O47-C7-C8	3.79	119.67	111.50
23	BV	601	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
24	BV	604	CLA	CHB-C1B-NB	3.79	128.26	124.26
23	BV	606	CHL	C3B-C4B-NB	3.78	114.03	110.52
23	BQ	607	CHL	CHB-C1B-NB	-3.78	120.25	124.26
25	BJ	616	LUT	C39-C29-C30	-3.78	117.62	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	8	307	CHL	CHB-C1B-NB	-3.78	120.25	124.26
23	r	606	CHL	O2D-CGD-CBD	3.78	117.99	111.27
23	G	607	CHL	C2D-C1D-ND	3.78	112.89	110.10
23	r	606	CHL	CAC-C3C-C4C	3.78	129.72	124.81
25	A2	615	LUT	C39-C29-C30	-3.78	117.63	122.92
28	r	616	XAT	C32-C33-C34	-3.78	113.14	118.94
23	Y	302	CHL	C1-C2-C3	-3.78	119.51	126.04
23	BQ	605	CHL	C3B-C4B-NB	3.77	114.02	110.52
23	S	601	CHL	CHB-C1B-NB	-3.77	120.26	124.26
23	e	601	CHL	C3B-C4B-NB	3.77	114.02	110.52
23	BH	601	CHL	C3B-C4B-NB	3.77	114.02	110.52
23	G	601	CHL	CAC-C3C-C4C	3.77	129.71	124.81
23	BH	601	CHL	C1D-ND-C4D	-3.77	103.66	106.33
23	9	609	CHL	C6-C5-C3	-3.77	108.45	114.62
23	BU	613	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	A2	615	LUT	C19-C9-C10	-3.77	117.64	122.92
23	r	613	CHL	CAC-C3C-C4C	3.77	129.70	124.81
23	6	608	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
32	l	102	SQD	O47-C7-C8	3.77	119.62	111.50
23	7	309	CHL	CHB-C1B-NB	-3.77	120.27	124.26
23	N	607	CHL	CAC-C3C-C4C	3.77	129.70	124.81
23	AA	309	CHL	CHB-C1B-NB	-3.77	120.27	124.26
23	BU	613	CHL	CHD-C4C-C3C	-3.77	119.31	124.84
23	BB	309	CHL	O2D-CGD-CBD	3.77	117.96	111.27
25	G	615	LUT	C39-C29-C30	-3.76	117.65	122.92
26	s	616	NEX	C15-C35-C34	3.76	131.18	123.47
23	Au	605	CHL	C3B-C4B-NB	3.76	114.01	110.52
32	BO	102	SQD	O47-C7-C8	3.76	119.61	111.50
23	AA	309	CHL	CAC-C3C-C4C	3.76	129.69	124.81
23	G	607	CHL	CAC-C3C-C4C	3.76	129.69	124.81
23	Ba	309	CHL	O2D-CGD-CBD	3.76	117.95	111.27
25	A6	614	LUT	C19-C9-C10	-3.76	117.66	122.92
28	AA	301	XAT	C32-C33-C34	-3.76	113.18	118.94
23	Au	605	CHL	CHD-C4C-C3C	-3.76	119.32	124.84
25	n	615	LUT	C19-C9-C10	-3.76	117.66	122.92
23	A6	605	CHL	C1D-ND-C4D	-3.76	103.67	106.33
23	BQ	601	CHL	CHD-C4C-C3C	-3.75	119.32	124.84
25	BJ	615	LUT	C39-C29-C30	-3.75	117.67	122.92
23	7	309	CHL	CHD-C4C-C3C	-3.75	119.32	124.84
24	6	602	CLA	C3B-C4B-NB	-3.75	107.03	110.52
25	BQ	615	LUT	C19-C9-C10	-3.75	117.67	122.92
23	BJ	601	CHL	C1D-ND-C4D	-3.75	103.67	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	615	LUT	C19-C9-C10	-3.75	117.67	122.92
28	BU	616	XAT	C38-C25-C24	-3.75	110.06	114.28
23	BV	605	CHL	CHD-C4C-C3C	-3.75	119.33	124.84
25	S	614	LUT	C39-C29-C30	-3.75	117.67	122.92
25	S	615	LUT	C39-C29-C30	-3.75	117.67	122.92
25	g	615	LUT	C39-C29-C30	-3.75	117.67	122.92
23	AA	309	CHL	C2D-C1D-ND	3.75	112.86	110.10
25	N	615	LUT	C39-C29-C30	-3.75	117.67	122.92
23	9	605	CHL	O2D-CGD-CBD	3.75	117.92	111.27
25	7	317	LUT	C15-C35-C34	3.75	131.15	123.47
23	7	309	CHL	C2D-C1D-ND	3.75	112.86	110.10
24	8	308	CLA	CMA-C3A-C4A	-3.74	101.71	111.77
23	AA	309	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
26	S	616	NEX	C15-C35-C34	3.74	131.14	123.47
23	n	601	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	A6	615	LUT	C39-C29-C30	-3.74	117.68	122.92
23	Au	609	CHL	CAC-C3C-C4C	3.74	129.66	124.81
32	BO	102	SQD	O7-S-C6	3.74	111.39	106.94
25	S	614	LUT	C19-C9-C10	-3.74	117.68	122.92
26	BV	616	NEX	C15-C35-C34	3.74	131.14	123.47
25	BJ	615	LUT	C35-C15-C14	3.74	131.13	123.47
23	N	607	CHL	C3B-C4B-NB	3.74	113.98	110.52
25	Au	615	LUT	C39-C29-C30	-3.74	117.69	122.92
23	S	601	CHL	C2D-C1D-ND	3.74	112.86	110.10
23	e	601	CHL	C1D-ND-C4D	-3.74	103.68	106.33
32	2	408	SQD	O9-S-O7	-3.74	101.02	113.95
25	6	615	LUT	C39-C29-C30	-3.73	117.69	122.92
23	Au	601	CHL	CHD-C4C-C3C	-3.73	119.35	124.84
32	BG	406	SQD	O9-S-C6	3.73	111.38	106.94
25	g	615	LUT	C35-C15-C14	3.73	131.12	123.47
34	BK	102	DGD	CDB-CCB-CBB	-3.73	95.49	114.42
32	L	103	SQD	O9-S-C6	3.73	111.37	106.94
23	6	601	CHL	CHB-C1B-NB	-3.73	120.31	124.26
23	0	601	CHL	CHB-C1B-NB	-3.73	120.31	124.26
25	A6	614	LUT	C39-C29-C30	-3.73	117.70	122.92
28	A2	619	XAT	C30-C31-C32	-3.73	111.59	123.22
28	7	318	XAT	C32-C33-C34	-3.73	113.22	118.94
23	S	606	CHL	CAC-C3C-C4C	3.72	129.64	124.81
25	Ba	317	LUT	C35-C15-C14	3.72	131.10	123.47
32	L	103	SQD	O7-S-C6	3.72	111.36	106.94
28	BU	616	XAT	C19-C9-C8	-3.72	112.22	118.08
28	7	301	XAT	C32-C33-C34	-3.72	113.23	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BQ	607	CHL	C2D-C1D-ND	3.72	112.84	110.10
26	BB	320	NEX	C35-C15-C14	3.72	131.09	123.47
32	A1	101	SQD	O9-S-C6	3.72	111.36	106.94
23	N	605	CHL	C2D-C1D-ND	3.72	112.84	110.10
23	g	606	CHL	CHB-C1B-NB	-3.72	120.32	124.26
28	N	619	XAT	C30-C31-C32	-3.71	111.63	123.22
23	y	302	CHL	C1-C2-C3	-3.71	119.62	126.04
23	s	606	CHL	CAC-C3C-C4C	3.71	129.63	124.81
23	5	606	CHL	C3B-C4B-NB	3.71	113.96	110.52
26	Au	617	NEX	C35-C15-C14	3.71	131.07	123.47
23	r	613	CHL	CHD-C4C-C3C	-3.71	119.39	124.84
25	AA	317	LUT	C15-C35-C34	3.71	131.07	123.47
23	n	605	CHL	C3B-C4B-NB	3.71	113.96	110.52
28	5	619	XAT	C10-C11-C12	-3.71	111.64	123.22
23	Y	309	CHL	C6-C5-C3	-3.71	108.56	114.62
23	0	608	CHL	CAC-C3C-C4C	3.71	129.62	124.81
23	6	609	CHL	CAC-C3C-C4C	3.70	129.62	124.81
23	A2	605	CHL	C2D-C1D-ND	3.70	112.83	110.10
26	G	617	NEX	C35-C15-C14	3.70	131.06	123.47
23	A2	607	CHL	CHB-C1B-NB	-3.70	120.34	124.26
32	Az	101	SQD	O47-C7-C8	3.70	119.48	111.50
25	y	317	LUT	C35-C15-C14	3.70	131.06	123.47
25	Y	316	LUT	C39-C29-C30	-3.70	117.74	122.92
23	AA	309	CHL	C3B-C4B-NB	3.70	113.95	110.52
23	Au	601	CHL	C2D-C1D-ND	3.70	112.83	110.10
23	N	607	CHL	CHB-C1B-NB	-3.70	120.34	124.26
23	5	601	CHL	CHB-C1B-NB	-3.70	120.34	124.26
24	BV	610	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
23	Y	307	CHL	C1D-ND-C4D	-3.70	103.71	106.33
23	Ba	308	CHL	C3B-C4B-NB	3.70	113.94	110.52
25	s	614	LUT	C39-C29-C30	-3.70	117.75	122.92
23	BJ	606	CHL	CHB-C1B-NB	-3.69	120.35	124.26
23	A2	601	CHL	CHB-C1B-NB	-3.69	120.35	124.26
24	b	611	CLA	CMC-C2C-C3C	3.69	136.14	126.12
25	Y	316	LUT	C15-C35-C34	3.69	131.04	123.47
23	A6	601	CHL	C2D-C1D-ND	3.69	112.82	110.10
32	A1	101	SQD	O9-S-O7	-3.69	101.18	113.95
23	G	601	CHL	C2D-C1D-ND	3.69	112.82	110.10
23	s	605	CHL	CHB-C1B-NB	-3.69	120.35	124.26
23	n	609	CHL	CHD-C4C-C3C	-3.69	119.42	124.84
23	BU	605	CHL	C2D-C1D-ND	3.69	112.82	110.10
23	BB	310	CHL	CHD-C4C-C3C	-3.68	119.42	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Y	306	CHL	CHD-C4C-C3C	-3.68	119.42	124.84
23	s	601	CHL	CHD-C4C-C3C	-3.68	119.42	124.84
26	BB	318	NEX	C19-C9-C10	-3.68	117.76	122.92
23	9	601	CHL	CHB-C1B-NB	-3.68	120.36	124.26
23	n	607	CHL	C2D-C1D-ND	3.68	112.82	110.10
23	g	608	CHL	C1D-ND-C4D	-3.68	103.72	106.33
23	y	306	CHL	CHD-C4C-C3C	-3.68	119.43	124.84
24	s	610	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
23	BB	306	CHL	CHD-C4C-C3C	-3.68	119.44	124.84
25	BV	614	LUT	C39-C29-C30	-3.68	117.77	122.92
26	A2	617	NEX	C20-C13-C14	-3.68	117.78	122.92
32	d	406	SQD	O9-S-O7	-3.67	101.23	113.95
23	6	607	CHL	C3B-C4B-NB	3.67	113.92	110.52
28	g	619	XAT	C30-C31-C32	-3.67	111.75	123.22
23	AB	305	CHL	CHD-C4C-C3C	-3.67	119.44	124.84
32	L	103	SQD	O9-S-O7	-3.67	101.25	113.95
23	BB	309	CHL	C6-C5-C3	-3.67	108.62	114.62
23	Y	309	CHL	C2D-C1D-ND	3.67	112.81	110.10
23	BU	606	CHL	CAC-C3C-C4C	3.67	129.57	124.81
32	BG	406	SQD	O9-S-O7	-3.67	101.26	113.95
25	6	615	LUT	C19-C9-C10	-3.67	117.79	122.92
25	AB	311	LUT	C32-C33-C34	3.67	124.56	118.94
23	BB	302	CHL	C3B-C4B-NB	3.66	113.92	110.52
25	G	616	LUT	C35-C15-C14	3.66	130.98	123.47
32	BD	412	SQD	O9-S-O7	-3.66	101.27	113.95
23	BB	308	CHL	CAC-C3C-C4C	3.66	129.56	124.81
23	A2	608	CHL	CAC-C3C-C4C	3.66	129.56	124.81
32	a	412	SQD	O9-S-O7	-3.66	101.28	113.95
23	Ba	306	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
23	s	605	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
28	BJ	619	XAT	C30-C31-C32	-3.66	111.80	123.22
23	9	608	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
23	n	605	CHL	CHB-C1B-NB	-3.66	120.39	124.26
25	r	615	LUT	C39-C29-C30	-3.66	117.80	122.92
31	d	403	PL9	C36-C34-C33	-3.65	113.73	121.12
23	BB	309	CHL	C2D-C1D-ND	3.65	112.79	110.10
23	6	607	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
25	AB	311	LUT	C39-C29-C30	-3.65	117.81	122.92
23	BB	307	CHL	C1D-ND-C4D	-3.65	103.75	106.33
23	BB	308	CHL	C1D-ND-C4D	-3.65	103.75	106.33
23	N	608	CHL	CAC-C3C-C4C	3.65	129.54	124.81
28	n	619	XAT	C12-C13-C14	-3.65	113.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	607	CHL	CHB-C1B-NB	-3.65	120.40	124.26
25	BB	316	LUT	C39-C29-C30	-3.64	117.82	122.92
26	y	318	NEX	C15-C35-C34	3.64	130.93	123.47
23	BQ	605	CHL	CHB-C1B-NB	-3.64	120.40	124.26
32	l	102	SQD	O7-S-C6	3.64	111.27	106.94
32	A	413	SQD	O9-S-O7	-3.64	101.35	113.95
26	BB	318	NEX	C15-C35-C34	3.64	130.93	123.47
28	n	619	XAT	C30-C31-C32	-3.64	111.86	123.22
23	5	608	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
23	5	601	CHL	C3B-C4B-NB	3.64	113.89	110.52
23	n	606	CHL	C2D-C1D-ND	3.64	112.78	110.10
23	BJ	601	CHL	CAC-C3C-C4C	3.63	129.53	124.81
23	8	305	CHL	CHD-C4C-C3C	-3.63	119.50	124.84
25	BQ	616	LUT	C35-C15-C14	3.63	130.92	123.47
23	A6	606	CHL	CAC-C3C-C4C	3.63	129.52	124.81
28	BQ	619	XAT	C30-C31-C32	-3.63	111.88	123.22
23	N	601	CHL	CHB-C1B-NB	-3.63	120.41	124.26
23	Y	309	CHL	O2D-CGD-CBD	3.63	117.72	111.27
32	R	411	SQD	O9-S-O7	-3.63	101.39	113.95
26	r	617	NEX	C19-C9-C10	-3.63	117.84	122.92
28	AA	318	XAT	C32-C33-C34	-3.63	113.37	118.94
34	1	517	DGD	O6D-C1D-O3G	-3.63	101.38	109.97
23	N	608	CHL	CHD-C4C-C3C	-3.63	119.51	124.84
23	y	308	CHL	C3B-C4B-NB	3.63	113.88	110.52
24	R	406	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
23	9	605	CHL	CHD-C4C-C3C	-3.62	119.51	124.84
23	n	608	CHL	CAC-C3C-C4C	3.62	129.51	124.81
24	BE	609	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	5	605	CHL	CHD-C4C-C3C	-3.62	119.52	124.84
23	8	307	CHL	C3B-C4B-NB	3.62	113.87	110.52
23	A2	606	CHL	C2D-C1D-ND	3.62	112.77	110.10
23	BQ	601	CHL	C2D-C1D-ND	3.62	112.77	110.10
23	Ba	302	CHL	CHD-C4C-C3C	-3.62	119.53	124.84
26	r	617	NEX	C15-C35-C34	3.61	130.88	123.47
23	y	308	CHL	CAC-C3C-C4C	3.61	129.50	124.81
34	BK	102	DGD	O3G-C3G-C2G	-3.61	102.18	110.90
23	Y	310	CHL	CHD-C4C-C3C	-3.61	119.53	124.84
23	Ba	302	CHL	CAC-C3C-C4C	3.61	129.50	124.81
23	BJ	608	CHL	C6-C5-C3	-3.61	108.72	114.62
28	y	301	XAT	C12-C13-C14	-3.61	113.40	118.94
26	S	616	NEX	C20-C13-C14	-3.61	117.87	122.92
25	9	615	LUT	C20-C13-C14	-3.61	117.87	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	601	CHL	C2D-C1D-ND	3.60	112.76	110.10
23	y	302	CHL	CHD-C4C-C3C	-3.60	119.55	124.84
25	BU	615	LUT	C39-C29-C30	-3.60	117.88	122.92
23	n	601	CHL	C2D-C1D-ND	3.60	112.76	110.10
23	Y	308	CHL	CAC-C3C-C4C	3.60	129.48	124.81
23	Y	302	CHL	C3B-C4B-NB	3.60	113.85	110.52
23	g	608	CHL	C6-C5-C3	-3.60	108.73	114.62
23	A2	608	CHL	CHD-C4C-C3C	-3.60	119.55	124.84
23	6	608	CHL	CAC-C3C-C4C	3.60	129.48	124.81
25	A6	614	LUT	C15-C35-C34	3.60	130.84	123.47
23	g	607	CHL	C3B-C4B-NB	3.59	113.85	110.52
23	Ba	309	CHL	C6-C5-C3	-3.59	108.74	114.62
23	y	309	CHL	CED-O2D-CGD	3.59	124.06	115.94
28	Au	619	XAT	C30-C31-C32	-3.59	112.01	123.22
23	Au	607	CHL	CHB-C1B-NB	-3.59	120.46	124.26
23	BV	601	CHL	CAC-C3C-C4C	3.59	129.47	124.81
32	L	101	SQD	O47-C7-C8	3.59	119.23	111.50
23	Y	309	CHL	CAC-C3C-C4C	3.59	129.47	124.81
23	BQ	608	CHL	CAC-C3C-C4C	3.59	129.47	124.81
25	A6	615	LUT	C15-C35-C34	3.59	130.82	123.47
28	Ba	301	XAT	C12-C13-C14	-3.59	113.44	118.94
28	9	619	XAT	C40-C33-C32	-3.59	112.43	118.08
25	S	615	LUT	C15-C35-C34	3.59	130.82	123.47
26	Ba	318	NEX	C15-C35-C34	3.58	130.81	123.47
23	Y	308	CHL	C1D-ND-C4D	-3.58	103.79	106.33
26	BJ	617	NEX	C19-C9-C10	-3.58	117.91	122.92
26	Ba	318	NEX	C20-C13-C14	-3.58	117.91	122.92
23	AA	308	CHL	C3B-C4B-NB	3.58	113.83	110.52
24	6	604	CLA	CAC-C3C-C2C	3.58	133.65	127.53
24	v	611	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
23	9	601	CHL	C3B-C4B-NB	3.58	113.83	110.52
23	A6	606	CHL	C3B-C4B-NB	3.58	113.83	110.52
26	Au	617	NEX	C20-C13-C14	-3.58	117.91	122.92
23	7	310	CHL	CAC-C3C-C4C	3.58	129.45	124.81
24	9	610	CLA	C3B-C4B-NB	-3.58	107.20	110.52
24	A	407	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
23	y	309	CHL	C6-C5-C3	-3.57	108.77	114.62
23	7	308	CHL	C3B-C4B-NB	3.57	113.83	110.52
23	Au	607	CHL	C3B-C4B-NB	3.57	113.83	110.52
23	y	302	CHL	CAC-C3C-C4C	3.57	129.45	124.81
28	r	616	XAT	C20-C13-C12	-3.57	112.45	118.08
28	G	619	XAT	C30-C31-C32	-3.57	112.07	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	309	CHL	CAC-C3C-C4C	3.57	129.44	124.81
26	A6	616	NEX	C15-C35-C34	3.57	130.79	123.47
23	5	609	CHL	C6-C5-C3	-3.57	108.78	114.62
23	BQ	608	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
23	g	601	CHL	CAC-C3C-C4C	3.57	129.44	124.81
26	BB	320	NEX	C15-C35-C34	3.57	130.79	123.47
26	y	318	NEX	C20-C13-C14	-3.57	117.92	122.92
32	A	413	SQD	O7-S-C6	3.57	111.18	106.94
32	l	101	SQD	O9-S-O7	-3.57	101.60	113.95
32	BO	101	SQD	O9-S-O7	-3.57	101.60	113.95
23	Au	608	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
34	C	517	DGD	O6D-C1D-O3G	-3.57	101.53	109.97
23	N	607	CHL	C1D-ND-C4D	-3.57	103.80	106.33
24	y	311	CLA	C1-C2-C3	-3.57	119.88	126.04
23	n	608	CHL	CHD-C4C-C3C	-3.57	119.60	124.84
32	A	413	SQD	O9-S-C6	3.57	111.18	106.94
26	G	617	NEX	C19-C9-C10	-3.57	117.93	122.92
23	BB	310	CHL	C3B-C4B-NB	3.56	113.82	110.52
28	y	301	XAT	C30-C31-C32	-3.56	112.09	123.22
24	BF	512	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
28	BU	616	XAT	C20-C13-C12	-3.56	112.46	118.08
26	G	617	NEX	C20-C13-C14	-3.56	117.93	122.92
28	BB	301	XAT	C10-C11-C12	-3.56	112.10	123.22
25	BV	614	LUT	C19-C9-C10	-3.56	117.93	122.92
23	g	606	CHL	C2D-C1D-ND	3.56	112.73	110.10
23	Au	601	CHL	CHB-C1B-NB	-3.56	120.49	124.26
23	Au	601	CHL	C1-C2-C3	-3.56	119.88	126.04
34	BK	102	DGD	CAB-C9B-C8B	-3.56	96.35	114.42
23	A2	601	CHL	C2D-C1D-ND	3.56	112.73	110.10
28	r	616	XAT	C10-C11-C12	-3.56	112.11	123.22
23	AA	306	CHL	C4A-NA-C1A	3.56	108.31	106.71
26	Au	617	NEX	C19-C9-C10	-3.56	117.94	122.92
25	s	615	LUT	C35-C15-C14	3.56	130.76	123.47
23	Y	310	CHL	C3B-C4B-NB	3.56	113.82	110.52
23	G	601	CHL	C1-C2-C3	-3.56	119.89	126.04
23	BV	606	CHL	CAC-C3C-C4C	3.56	129.43	124.81
28	Y	301	XAT	C28-C29-C30	-3.56	113.48	118.94
23	N	601	CHL	CAC-C3C-C4C	3.56	129.42	124.81
29	b	601	BCR	C2-C1-C6	3.56	115.95	110.48
23	S	606	CHL	C3B-C4B-NB	3.55	113.81	110.52
32	Az	101	SQD	O8-S-C6	3.55	111.41	105.74
28	Y	301	XAT	C10-C11-C12	-3.55	112.13	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A2	619	XAT	C10-C11-C12	-3.55	112.14	123.22
23	y	306	CHL	O2D-CGD-CBD	3.55	117.58	111.27
26	A6	616	NEX	C20-C13-C14	-3.55	117.95	122.92
25	BV	615	LUT	C35-C15-C14	3.55	130.74	123.47
23	7	308	CHL	C6-C5-C3	-3.55	108.82	114.62
28	Ba	301	XAT	C30-C31-C32	-3.54	112.16	123.22
28	8	312	XAT	C32-C33-C34	-3.54	113.50	118.94
23	Au	609	CHL	C2D-C1D-ND	3.54	112.72	110.10
26	g	617	NEX	C19-C9-C10	-3.54	117.96	122.92
23	AB	307	CHL	CMD-C2D-C3D	-3.54	119.47	127.61
23	BU	613	CHL	C2D-C1D-ND	3.54	112.71	110.10
28	BB	301	XAT	C28-C29-C30	-3.54	113.51	118.94
23	y	310	CHL	CHC-C4B-NB	-3.54	120.51	124.26
28	9	619	XAT	C30-C31-C32	-3.54	112.17	123.22
32	R	411	SQD	O9-S-C6	3.54	111.14	106.94
23	A2	601	CHL	CAC-C3C-C4C	3.54	129.40	124.81
23	BQ	608	CHL	C3B-C4B-NB	3.54	113.80	110.52
23	Ba	310	CHL	CHC-C4B-NB	-3.53	120.52	124.26
32	BG	406	SQD	O7-S-C6	3.53	111.14	106.94
26	Y	318	NEX	C15-C35-C34	3.53	130.71	123.47
26	7	319	NEX	C20-C13-C14	-3.53	117.97	122.92
26	N	617	NEX	C20-C13-C14	-3.53	117.97	122.92
28	Ba	301	XAT	C10-C11-C12	-3.53	112.19	123.22
28	BU	616	XAT	C10-C11-C12	-3.53	112.20	123.22
23	Ba	309	CHL	CAC-C3C-C4C	3.53	129.39	124.81
23	s	601	CHL	CAC-C3C-C4C	3.53	129.39	124.81
23	AB	305	CHL	CAC-C3C-C4C	3.53	129.39	124.81
23	r	613	CHL	C3B-C4B-NB	3.53	113.79	110.52
23	r	613	CHL	C3D-C4D-ND	3.53	115.95	110.24
23	AA	310	CHL	CAC-C3C-C4C	3.53	129.39	124.81
23	8	305	CHL	CAC-C3C-C4C	3.53	129.39	124.81
23	BJ	607	CHL	C1D-ND-C4D	-3.53	103.83	106.33
23	BJ	608	CHL	C1D-ND-C4D	-3.53	103.83	106.33
23	BJ	606	CHL	C2D-C1D-ND	3.53	112.70	110.10
23	5	607	CHL	CAC-C3C-C4C	3.53	129.38	124.81
23	G	605	CHL	C3B-C4B-NB	3.52	113.78	110.52
23	BV	605	CHL	CHB-C1B-NB	-3.52	120.53	124.26
23	s	607	CHL	C2D-C1D-ND	3.52	112.70	110.10
23	BV	607	CHL	C2D-C1D-ND	3.52	112.70	110.10
26	s	616	NEX	C40-C33-C34	-3.52	117.99	122.92
23	G	608	CHL	CHD-C4C-C3C	-3.52	119.66	124.84
24	B	611	CLA	O2D-CGD-O1D	-3.52	116.95	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	L	101	SQD	O9-S-O7	-3.52	101.76	113.95
23	BQ	609	CHL	CHD-C4C-C3C	-3.52	119.67	124.84
23	7	307	CHL	C3B-C4B-NB	3.52	113.78	110.52
23	Ba	306	CHL	O2D-CGD-CBD	3.52	117.52	111.27
23	AA	308	CHL	C1D-ND-C4D	-3.52	103.83	106.33
25	s	614	LUT	C19-C9-C10	-3.52	118.00	122.92
26	AA	319	NEX	C20-C13-C14	-3.52	118.00	122.92
28	Y	301	XAT	C32-C33-C34	-3.52	113.54	118.94
28	AB	312	XAT	C32-C33-C34	-3.52	113.54	118.94
26	n	617	NEX	C20-C13-C14	-3.52	118.00	122.92
23	9	606	CHL	C3B-C4B-NB	3.52	113.78	110.52
23	y	309	CHL	CAC-C3C-C4C	3.52	129.37	124.81
29	BE	601	BCR	C2-C1-C6	3.52	115.89	110.48
23	7	308	CHL	C1D-ND-C4D	-3.51	103.84	106.33
28	N	619	XAT	C10-C11-C12	-3.51	112.25	123.22
23	Y	306	CHL	O2D-CGD-CBD	3.51	117.51	111.27
23	5	607	CHL	C3B-C4B-NB	3.51	113.77	110.52
32	D	406	SQD	O7-S-C6	3.51	111.11	106.94
32	R	411	SQD	O7-S-C6	3.51	111.11	106.94
23	Ba	302	CHL	C2D-C1D-ND	3.51	112.69	110.10
23	r	613	CHL	CHB-C1B-NB	-3.51	120.54	124.26
25	6	616	LUT	C40-C33-C34	-3.51	118.01	122.92
23	S	606	CHL	CHB-C1B-NB	-3.51	120.55	124.26
23	A2	607	CHL	C1D-ND-C4D	-3.51	103.84	106.33
23	8	305	CHL	C3B-C4B-NB	3.50	113.77	110.52
23	9	607	CHL	CHB-C1B-NB	-3.50	120.55	124.26
23	Au	607	CHL	C1D-ND-C4D	-3.50	103.85	106.33
23	y	308	CHL	C1D-ND-C4D	-3.50	103.85	106.33
28	y	301	XAT	C10-C11-C12	-3.50	112.30	123.22
23	N	606	CHL	C2D-C1D-ND	3.50	112.68	110.10
32	BO	101	SQD	O7-S-C6	3.50	111.09	106.94
23	BB	306	CHL	O2D-CGD-CBD	3.50	117.48	111.27
23	BQ	606	CHL	CMB-C2B-C1B	3.50	130.69	125.37
23	g	607	CHL	C1D-ND-C4D	-3.49	103.85	106.33
23	BJ	607	CHL	C3B-C4B-NB	3.49	113.76	110.52
23	G	606	CHL	C2D-C1D-ND	3.49	112.68	110.10
26	BB	318	NEX	C12-C13-C14	3.49	124.30	118.94
23	BU	606	CHL	C3B-C4B-NB	3.49	113.75	110.52
24	BQ	610	CLA	CMA-C3A-C4A	-3.49	102.40	111.77
23	G	607	CHL	CHB-C1B-NB	-3.49	120.56	124.26
23	AA	308	CHL	C4-C3-C5	3.49	121.14	115.27
24	6	610	CLA	C3B-C4B-NB	-3.49	107.28	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Au	605	CHL	CAC-C3C-C4C	3.49	129.33	124.81
34	BF	518	DGD	O6D-C1D-O3G	-3.49	101.72	109.97
28	n	619	XAT	C19-C9-C8	-3.49	112.58	118.08
28	BQ	619	XAT	C19-C9-C8	-3.48	112.59	118.08
25	Ba	316	LUT	C15-C35-C34	3.48	130.61	123.47
24	8	308	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
23	6	605	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
23	s	606	CHL	C1D-ND-C4D	-3.48	103.86	106.33
23	9	608	CHL	C3B-C4B-NB	3.48	113.74	110.52
25	S	614	LUT	C15-C35-C34	3.48	130.60	123.47
32	l	101	SQD	O9-S-C6	3.47	111.07	106.94
23	n	607	CHL	CAC-C3C-C4C	3.47	129.32	124.81
23	Ba	308	CHL	CHB-C1B-NB	-3.47	120.58	124.26
23	AA	307	CHL	C3B-C4B-NB	3.47	113.74	110.52
24	A6	609	CLA	C3B-C4B-NB	-3.47	107.29	110.52
23	5	606	CHL	C1D-ND-C4D	-3.47	103.87	106.33
26	N	617	NEX	C12-C13-C14	3.47	124.27	118.94
23	N	606	CHL	CAC-C3C-C4C	3.47	129.31	124.81
26	BB	318	NEX	C20-C13-C14	-3.47	118.06	122.92
26	BV	616	NEX	C40-C33-C34	-3.47	118.06	122.92
23	Au	606	CHL	C2D-C1D-ND	3.47	112.66	110.10
23	BU	613	CHL	C3D-C4D-ND	3.47	115.85	110.24
23	G	606	CHL	CHB-C1B-NB	-3.47	120.58	124.26
23	AB	304	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
23	0	609	CHL	CMD-C2D-C3D	-3.47	119.64	127.61
26	7	319	NEX	C19-C9-C10	-3.47	118.07	122.92
25	BQ	615	LUT	C35-C15-C14	3.47	130.57	123.47
23	BV	606	CHL	CHB-C1B-NB	-3.46	120.59	124.26
23	6	605	CHL	CAC-C3C-C4C	3.46	129.31	124.81
34	a	401	DGD	O6D-C1D-O3G	-3.46	101.77	109.97
23	r	606	CHL	C3B-C4B-NB	3.46	113.73	110.52
32	2	408	SQD	O7-S-C6	3.46	111.06	106.94
32	BO	101	SQD	O9-S-C6	3.46	111.06	106.94
34	c	516	DGD	O6D-C1D-O3G	-3.46	101.77	109.97
28	BB	301	XAT	C32-C33-C34	-3.46	113.63	118.94
26	BJ	617	NEX	C20-C13-C14	-3.46	118.07	122.92
23	BU	613	CHL	C1D-ND-C4D	-3.46	103.88	106.33
23	5	606	CHL	C2D-C1D-ND	3.46	112.65	110.10
23	0	607	CHL	CHD-C4C-C3C	-3.46	119.76	124.84
23	AB	305	CHL	C3B-C4B-NB	3.46	113.72	110.52
23	BV	601	CHL	C2D-C1D-ND	3.46	112.65	110.10
23	G	601	CHL	CHB-C1B-NB	-3.46	120.60	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ba	302	CHL	C1-C2-C3	-3.46	120.06	126.04
23	n	608	CHL	C3B-C4B-NB	3.46	113.72	110.52
23	AA	302	CHL	CAC-C3C-C4C	3.46	129.29	124.81
32	l	101	SQD	O7-S-C6	3.45	111.05	106.94
23	Y	302	CHL	C1D-ND-C4D	-3.45	103.88	106.33
23	S	605	CHL	C3B-C4B-NB	3.45	113.72	110.52
34	BD	413	DGD	O6D-C1D-O3G	-3.45	101.80	109.97
23	y	308	CHL	CHB-C1B-NB	-3.45	120.60	124.26
24	0	613	CLA	C1-C2-C3	-3.45	120.07	126.04
23	e	601	CHL	C3D-C4D-ND	3.45	115.82	110.24
23	s	601	CHL	C2D-C1D-ND	3.45	112.65	110.10
23	7	302	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
23	5	608	CHL	C3B-C4B-NB	3.45	113.72	110.52
23	BH	601	CHL	C3D-C4D-ND	3.45	115.82	110.24
23	BQ	601	CHL	C3B-C4B-NB	3.45	113.71	110.52
28	y	301	XAT	C19-C9-C8	-3.45	112.64	118.08
24	0	610	CLA	C3B-C4B-NB	-3.45	107.32	110.52
25	n	615	LUT	C35-C15-C14	3.45	130.53	123.47
26	s	616	NEX	C20-C13-C14	-3.45	118.09	122.92
26	BB	318	NEX	C40-C33-C34	-3.45	118.09	122.92
23	Au	608	CHL	C3B-C4B-NB	3.45	113.71	110.52
23	n	607	CHL	C6-C5-C3	-3.45	108.98	114.62
23	Au	606	CHL	CHB-C1B-NB	-3.44	120.61	124.26
24	AA	311	CLA	C3B-C4B-NB	-3.44	107.32	110.52
23	A6	606	CHL	CHB-C1B-NB	-3.44	120.61	124.26
23	G	608	CHL	C3B-C4B-NB	3.44	113.71	110.52
23	Y	309	CHL	C3B-C4B-NB	3.44	113.71	110.52
23	BU	613	CHL	C3B-C4B-NB	3.44	113.71	110.52
23	n	606	CHL	CMB-C2B-C1B	3.44	130.61	125.37
26	n	617	NEX	C40-C33-C34	-3.44	118.11	122.92
26	A2	617	NEX	C40-C33-C34	-3.44	118.11	122.92
23	n	601	CHL	C3B-C4B-NB	3.44	113.70	110.52
23	Au	609	CHL	CHB-C1B-NB	-3.44	120.62	124.26
26	N	617	NEX	C40-C33-C34	-3.44	118.11	122.92
23	BB	302	CHL	C1D-ND-C4D	-3.43	103.89	106.33
24	BG	401	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
26	BQ	617	NEX	C19-C9-C10	-3.43	118.11	122.92
28	Ba	301	XAT	C19-C9-C8	-3.43	112.67	118.08
26	BQ	617	NEX	C40-C33-C34	-3.43	118.11	122.92
24	6	611	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
23	0	605	CHL	CAC-C3C-C4C	3.43	129.26	124.81
23	BB	307	CHL	C3B-C4B-NB	3.43	113.70	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	617	NEX	C20-C13-C14	-3.43	118.12	122.92
26	AA	319	NEX	C19-C9-C10	-3.43	118.12	122.92
28	r	616	XAT	C18-C5-C4	-3.43	110.42	114.28
34	c	517	DGD	O6D-C1D-O3G	-3.43	101.86	109.97
26	y	318	NEX	C40-C33-C34	-3.43	118.12	122.92
34	a	413	DGD	O6D-C1D-O3G	-3.43	101.86	109.97
23	y	307	CHL	C2D-C1D-ND	3.43	112.63	110.10
23	BU	613	CHL	CHB-C1B-NB	-3.43	120.63	124.26
26	BV	616	NEX	C20-C13-C14	-3.43	118.12	122.92
23	AA	308	CHL	C1-C2-C3	-3.42	120.12	126.04
34	BF	517	DGD	O6D-C1D-O3G	-3.42	101.86	109.97
23	9	601	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
23	r	613	CHL	C2D-C1D-ND	3.42	112.63	110.10
23	r	613	CHL	C1D-ND-C4D	-3.42	103.90	106.33
28	8	312	XAT	C30-C31-C32	-3.42	112.53	123.22
26	5	617	NEX	C20-C13-C14	-3.42	118.13	122.92
23	5	606	CHL	CMB-C2B-C1B	3.42	130.58	125.37
28	AB	312	XAT	C30-C31-C32	-3.42	112.54	123.22
28	A2	619	XAT	C20-C13-C12	-3.42	112.69	118.08
23	A2	606	CHL	CAC-C3C-C4C	3.42	129.25	124.81
23	0	605	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
26	9	617	NEX	C20-C13-C14	-3.42	118.13	122.92
25	Y	317	LUT	C35-C15-C14	3.42	130.48	123.47
34	C	516	DGD	O6D-C1D-O3G	-3.42	101.88	109.97
23	Y	307	CHL	C3B-C4B-NB	3.42	113.69	110.52
23	9	609	CHL	C3B-C4B-NB	3.42	113.69	110.52
23	BV	606	CHL	C1D-ND-C4D	-3.42	103.91	106.33
26	BB	320	NEX	C40-C33-C34	-3.42	118.14	122.92
28	7	318	XAT	C30-C31-C32	-3.42	112.56	123.22
23	G	607	CHL	C1D-ND-C4D	-3.42	103.91	106.33
23	A6	605	CHL	C3B-C4B-NB	3.42	113.68	110.52
25	0	616	LUT	C40-C33-C34	-3.41	118.14	122.92
23	AA	310	CHL	C6-C5-C3	-3.41	109.04	114.62
23	r	607	CHL	CHB-C1B-NB	-3.41	120.65	124.26
23	8	305	CHL	C2D-C1D-ND	3.41	112.62	110.10
23	8	304	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
26	BJ	617	NEX	C40-C33-C34	-3.41	118.15	122.92
23	5	601	CHL	C1D-ND-C4D	-3.41	103.91	106.33
34	BD	401	DGD	O6D-C1D-O3G	-3.41	101.91	109.97
23	S	605	CHL	C3D-C4D-ND	3.41	115.75	110.24
34	1	516	DGD	O6D-C1D-O3G	-3.41	101.91	109.97
23	s	606	CHL	CHB-C1B-NB	-3.41	120.65	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	601	CHL	C1-C2-C3	-3.41	120.15	126.04
23	y	306	CHL	C2D-C1D-ND	3.41	112.61	110.10
26	Y	318	NEX	C40-C33-C34	-3.40	118.15	122.92
26	r	617	NEX	C40-C33-C34	-3.40	118.15	122.92
23	g	601	CHL	C3D-C4D-ND	3.40	115.75	110.24
23	7	302	CHL	CAC-C3C-C4C	3.40	129.23	124.81
28	Y	301	XAT	C30-C31-C32	-3.40	112.60	123.22
23	AB	306	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
23	6	609	CHL	C1-C2-C3	-3.40	120.16	126.04
23	g	605	CHL	CHB-C1B-NB	-3.40	120.66	124.26
23	N	608	CHL	C3B-C4B-NB	3.40	113.67	110.52
23	7	308	CHL	CAC-C3C-C4C	3.40	129.22	124.81
23	8	307	CHL	CAC-C3C-C4C	3.40	129.22	124.81
23	Au	601	CHL	C1D-ND-C4D	-3.40	103.92	106.33
26	BQ	617	NEX	C20-C13-C14	-3.40	118.16	122.92
28	g	619	XAT	C10-C11-C12	-3.40	112.61	123.22
23	N	601	CHL	C1D-ND-C4D	-3.40	103.92	106.33
23	Ba	308	CHL	C1D-ND-C4D	-3.40	103.92	106.33
26	9	617	NEX	C40-C33-C34	-3.40	118.16	122.92
23	BQ	607	CHL	C6-C5-C3	-3.40	109.06	114.62
23	BJ	605	CHL	CHB-C1B-NB	-3.40	120.66	124.26
23	Ba	306	CHL	C2D-C1D-ND	3.40	112.61	110.10
28	AA	318	XAT	C30-C31-C32	-3.40	112.62	123.22
28	BB	301	XAT	C30-C31-C32	-3.39	112.63	123.22
23	BH	601	CHL	CAC-C3C-C4C	3.39	129.21	124.81
25	5	615	LUT	C20-C13-C14	-3.39	118.17	122.92
23	g	608	CHL	C3D-C4D-ND	3.39	115.72	110.24
23	BJ	601	CHL	C3D-C4D-ND	3.39	115.72	110.24
28	8	312	XAT	C18-C5-C4	-3.39	110.47	114.28
28	BU	616	XAT	C18-C5-C4	-3.39	110.47	114.28
26	5	617	NEX	C40-C33-C34	-3.39	118.17	122.92
23	Y	308	CHL	CHB-C1B-NB	-3.39	120.67	124.26
28	g	619	XAT	C12-C13-C14	-3.39	113.74	118.94
25	AB	311	LUT	C40-C33-C34	-3.39	118.18	122.92
28	7	318	XAT	C10-C11-C12	-3.39	112.64	123.22
23	AA	302	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
23	r	605	CHL	CMB-C2B-C1B	3.39	130.53	125.37
23	9	607	CHL	CAC-C3C-C4C	3.39	129.21	124.81
23	g	605	CHL	C3D-C4D-ND	3.39	115.72	110.24
28	BJ	619	XAT	C10-C11-C12	-3.39	112.65	123.22
28	BJ	619	XAT	C19-C9-C8	-3.39	112.74	118.08
23	N	609	CHL	C3B-C4B-NB	3.38	113.65	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	605	CHL	CAC-C3C-C4C	3.38	129.20	124.81
34	1	518	DGD	O6D-C1D-O3G	-3.38	101.97	109.97
23	5	601	CHL	CHD-C4C-C3C	-3.38	119.87	124.84
25	0	615	LUT	C39-C29-C30	-3.38	118.19	122.92
23	AA	308	CHL	CAC-C3C-C4C	3.38	129.19	124.81
28	AA	318	XAT	C20-C13-C12	-3.38	112.76	118.08
28	AA	318	XAT	C10-C11-C12	-3.38	112.68	123.22
23	r	606	CHL	CHD-C4C-C3C	-3.38	119.88	124.84
23	Ba	307	CHL	C2D-C1D-ND	3.38	112.59	110.10
23	Au	606	CHL	C3B-C4B-NB	3.38	113.65	110.52
34	C	518	DGD	O6D-C1D-O3G	-3.38	101.98	109.97
26	Ba	318	NEX	C40-C33-C34	-3.38	118.19	122.92
23	Ba	308	CHL	CAC-C3C-C4C	3.37	129.19	124.81
25	9	615	LUT	C12-C13-C14	3.37	124.12	118.94
23	A2	605	CHL	CAC-C3C-C4C	3.37	129.19	124.81
26	9	617	NEX	C32-C33-C34	3.37	124.12	118.94
28	g	619	XAT	C19-C9-C8	-3.37	112.76	118.08
32	d	406	SQD	O7-S-C6	3.37	110.95	106.94
24	BU	604	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
26	Y	318	NEX	C20-C13-C14	-3.37	118.20	122.92
28	AA	301	XAT	C20-C13-C12	-3.37	112.77	118.08
23	9	606	CHL	C3D-C4D-ND	3.37	115.69	110.24
23	BU	606	CHL	CHD-C4C-C3C	-3.37	119.89	124.84
23	g	601	CHL	C1-C2-C3	-3.37	120.22	126.04
25	s	614	LUT	C35-C15-C14	3.37	130.37	123.47
23	G	607	CHL	CMB-C2B-C1B	3.37	130.50	125.37
24	0	611	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
24	n	610	CLA	CMA-C3A-C4A	-3.37	102.72	111.77
24	8	308	CLA	CHB-C4A-NA	3.37	129.17	124.51
23	Y	302	CHL	C3D-C4D-ND	3.37	115.68	110.24
25	G	615	LUT	C40-C33-C34	-3.37	118.21	122.92
24	S	609	CLA	C3B-C4B-NB	-3.37	107.39	110.52
24	BB	315	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
23	A2	608	CHL	C3B-C4B-NB	3.36	113.63	110.52
23	BJ	608	CHL	C3D-C4D-ND	3.36	115.67	110.24
23	G	605	CHL	C1D-ND-C4D	-3.36	103.95	106.33
23	e	601	CHL	CAC-C3C-C4C	3.36	129.17	124.81
23	8	306	CHL	CHD-C4C-C3C	-3.36	119.90	124.84
23	BJ	605	CHL	C3D-C4D-ND	3.36	115.67	110.24
23	BQ	607	CHL	CAC-C3C-C4C	3.36	129.17	124.81
23	A6	605	CHL	C3D-C4D-ND	3.36	115.67	110.24
24	G	611	CLA	CED-O2D-CGD	3.35	123.52	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Au	615	LUT	C40-C33-C34	-3.35	118.22	122.92
23	r	605	CHL	C6-C5-C3	-3.35	109.14	114.62
25	Y	317	LUT	C20-C13-C14	-3.35	118.23	122.92
25	y	316	LUT	C20-C13-C14	-3.35	118.23	122.92
26	9	617	NEX	C19-C9-C10	-3.35	118.23	122.92
23	G	607	CHL	C3B-C4B-NB	3.35	113.62	110.52
23	A2	609	CHL	C3B-C4B-NB	3.35	113.62	110.52
23	7	306	CHL	C4A-NA-C1A	3.35	108.21	106.71
25	5	616	LUT	C35-C15-C14	3.35	130.34	123.47
25	9	616	LUT	C8-C9-C10	3.35	124.08	118.94
23	y	306	CHL	CAC-C3C-C4C	3.35	129.15	124.81
23	0	601	CHL	CHD-C4C-C3C	-3.35	119.92	124.84
23	9	607	CHL	C2D-C1D-ND	3.35	112.57	110.10
26	AA	319	NEX	C40-C33-C34	-3.35	118.23	122.92
28	n	619	XAT	C10-C11-C12	-3.35	112.77	123.22
23	9	601	CHL	C1D-ND-C4D	-3.35	103.96	106.33
28	BB	301	XAT	C20-C13-C12	-3.35	112.81	118.08
23	BU	607	CHL	CHB-C1B-NB	-3.34	120.72	124.26
24	AB	308	CLA	C3B-C4B-NB	-3.34	107.41	110.52
23	BU	605	CHL	CMB-C2B-C1B	3.34	130.46	125.37
25	AB	311	LUT	C20-C13-C14	-3.34	118.24	122.92
23	8	307	CHL	CHD-C4C-C3C	-3.34	119.92	124.84
23	BQ	606	CHL	C2D-C1D-ND	3.34	112.57	110.10
26	g	617	NEX	C40-C33-C34	-3.34	118.24	122.92
24	BU	608	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
26	Ba	318	NEX	C12-C13-C14	3.34	124.07	118.94
23	Ba	306	CHL	CAC-C3C-C4C	3.34	129.15	124.81
23	5	606	CHL	C3D-C4D-ND	3.34	115.64	110.24
24	BF	506	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
28	Y	301	XAT	C20-C13-C12	-3.34	112.81	118.08
31	d	403	PL9	C7-C3-C2	-3.34	118.91	123.30
28	N	619	XAT	C20-C13-C12	-3.34	112.82	118.08
28	BJ	619	XAT	C12-C13-C14	-3.34	113.82	118.94
28	AB	312	XAT	C18-C5-C4	-3.34	110.53	114.28
23	G	609	CHL	C1C-C2C-C3C	-3.34	104.47	107.11
23	AA	309	CHL	C1D-ND-C4D	-3.34	103.96	106.33
23	8	306	CHL	C4A-NA-C1A	3.34	108.21	106.71
23	5	606	CHL	CMD-C2D-C3D	-3.34	119.94	127.61
23	Au	601	CHL	C3D-C4D-ND	3.33	115.63	110.24
23	7	310	CHL	C6-C5-C3	-3.33	109.17	114.62
23	y	302	CHL	C2D-C1D-ND	3.33	112.56	110.10
28	8	312	XAT	C19-C9-C8	-3.33	112.83	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BQ	609	CHL	C1C-C2C-C3C	-3.33	104.47	107.11
23	N	601	CHL	C3D-C4D-ND	3.33	115.62	110.24
24	d	401	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
23	9	606	CHL	CMB-C2B-C1B	3.33	130.44	125.37
23	Au	607	CHL	CMB-C2B-C1B	3.33	130.44	125.37
23	n	605	CHL	C1D-ND-C4D	-3.33	103.97	106.33
26	y	318	NEX	C12-C13-C14	3.33	124.05	118.94
26	r	617	NEX	C20-C13-C14	-3.33	118.26	122.92
23	7	307	CHL	C2D-C1D-ND	3.33	112.56	110.10
24	6	610	CLA	CMA-C3A-C2A	-3.33	100.41	113.83
23	0	609	CHL	C1-C2-C3	-3.33	120.29	126.04
23	7	308	CHL	CHB-C1B-NB	-3.33	120.74	124.26
23	N	609	CHL	CMD-C2D-C3D	-3.33	119.96	127.61
23	BB	309	CHL	C3B-C4B-NB	3.33	113.60	110.52
23	BJ	606	CHL	C3B-C4B-NB	3.33	113.60	110.52
23	BB	306	CHL	CMB-C2B-C1B	3.32	130.43	125.37
28	7	301	XAT	C20-C13-C12	-3.32	112.84	118.08
34	R	401	DGD	O6D-C1D-O3G	-3.32	102.11	109.97
26	Au	617	NEX	C40-C33-C34	-3.32	118.27	122.92
23	A2	609	CHL	CMD-C2D-C3D	-3.32	119.97	127.61
23	A2	609	CHL	CAC-C3C-C4C	3.32	129.12	124.81
23	G	606	CHL	C3B-C4B-NB	3.32	113.59	110.52
23	6	601	CHL	CHD-C4C-C3C	-3.32	119.96	124.84
26	5	617	NEX	C32-C33-C34	3.32	124.03	118.94
23	BQ	601	CHL	CAC-C3C-C4C	3.32	129.12	124.81
28	BU	616	XAT	C40-C33-C32	-3.32	112.85	118.08
23	AB	305	CHL	C2D-C1D-ND	3.32	112.55	110.10
23	BJ	609	CHL	CMD-C2D-C3D	-3.32	119.98	127.61
25	Au	615	LUT	C20-C13-C14	-3.32	118.28	122.92
34	A	402	DGD	O6D-C1D-O3G	-3.32	102.12	109.97
23	Y	306	CHL	C2D-C1D-ND	3.32	112.55	110.10
24	A6	613	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	g	607	CHL	C3D-C4D-ND	3.31	115.60	110.24
23	AA	308	CHL	C3D-C4D-ND	3.31	115.60	110.24
26	G	617	NEX	C40-C33-C34	-3.31	118.28	122.92
24	Y	315	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	G	609	CHL	CHC-C4B-NB	-3.31	120.75	124.26
23	G	601	CHL	C1D-ND-C4D	-3.31	103.98	106.33
23	BB	308	CHL	CHB-C1B-NB	-3.31	120.75	124.26
23	G	607	CHL	C3D-C4D-ND	3.31	115.59	110.24
25	BB	317	LUT	C35-C15-C14	3.31	130.26	123.47
26	S	616	NEX	C19-C9-C10	-3.31	118.29	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	318	NEX	C12-C13-C14	3.31	124.02	118.94
28	7	318	XAT	C20-C13-C12	-3.31	112.87	118.08
23	n	605	CHL	CAC-C3C-C4C	3.31	129.10	124.81
23	6	609	CHL	CMD-C2D-C3D	-3.31	120.01	127.61
26	7	319	NEX	C40-C33-C34	-3.31	118.29	122.92
23	BB	306	CHL	C2D-C1D-ND	3.30	112.54	110.10
23	6	601	CHL	C2D-C1D-ND	3.30	112.54	110.10
23	BV	605	CHL	C3D-C4D-ND	3.30	115.58	110.24
28	7	301	XAT	C30-C31-C32	-3.30	112.91	123.22
24	1	511	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
26	S	616	NEX	C40-C33-C34	-3.30	118.30	122.92
28	7	301	XAT	C39-C29-C28	-3.30	112.88	118.08
24	9	602	CLA	C3B-C4B-NB	-3.30	107.45	110.52
24	b	609	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
23	9	606	CHL	CMD-C2D-C3D	-3.30	120.02	127.61
28	AA	301	XAT	C39-C29-C28	-3.30	112.88	118.08
29	BE	618	BCR	C30-C25-C26	-3.30	117.97	122.61
34	H	102	DGD	O3G-C3G-C2G	-3.30	102.94	110.90
23	BQ	607	CHL	C1D-ND-C4D	-3.30	103.99	106.33
26	9	617	NEX	C12-C13-C14	3.30	124.00	118.94
23	BQ	608	CHL	C2D-C1D-ND	3.30	112.53	110.10
23	BB	308	CHL	CMB-C2B-C1B	3.30	130.39	125.37
28	r	616	XAT	C40-C33-C32	-3.30	112.88	118.08
23	s	605	CHL	CMD-C2D-C3D	-3.30	120.03	127.61
23	BJ	607	CHL	C3D-C4D-ND	3.30	115.57	110.24
25	G	615	LUT	C20-C13-C14	-3.30	118.31	122.92
23	AA	308	CHL	CHB-C1B-NB	-3.30	120.77	124.26
23	6	607	CHL	C2D-C1D-ND	3.29	112.53	110.10
29	B	617	BCR	C15-C16-C17	-3.29	116.73	123.47
23	BB	302	CHL	C3D-C4D-ND	3.29	115.56	110.24
28	AA	301	XAT	C30-C31-C32	-3.29	112.95	123.22
26	Y	318	NEX	C19-C9-C10	-3.29	118.31	122.92
23	9	609	CHL	CAC-C3C-C4C	3.29	129.08	124.81
23	Au	609	CHL	C3D-C4D-ND	3.29	115.56	110.24
23	0	601	CHL	C2D-C1D-ND	3.29	112.53	110.10
23	G	601	CHL	C3D-C4D-ND	3.29	115.56	110.24
25	7	317	LUT	C20-C13-C14	-3.29	118.32	122.92
23	g	606	CHL	C3B-C4B-NB	3.29	113.56	110.52
23	7	308	CHL	C3D-C4D-ND	3.29	115.56	110.24
23	n	601	CHL	CAC-C3C-C4C	3.29	129.07	124.81
23	7	309	CHL	C1D-ND-C4D	-3.29	104.00	106.33
25	5	616	LUT	C20-C13-C14	-3.29	118.32	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	307	CHL	C2D-C1D-ND	3.29	112.53	110.10
28	BQ	619	XAT	C10-C11-C12	-3.29	112.96	123.22
28	AB	312	XAT	C39-C29-C28	-3.29	112.90	118.08
23	s	605	CHL	C3D-C4D-ND	3.28	115.55	110.24
23	BV	601	CHL	C3D-C4D-ND	3.28	115.55	110.24
23	BQ	605	CHL	C1D-ND-C4D	-3.28	104.00	106.33
23	9	609	CHL	C1-C2-C3	-3.28	120.37	126.04
23	BB	306	CHL	C3B-C4B-NB	3.28	113.56	110.52
26	A6	616	NEX	C19-C9-C10	-3.28	118.33	122.92
23	9	605	CHL	C2D-C1D-ND	3.28	112.52	110.10
23	BB	308	CHL	C4-C3-C5	3.28	120.79	115.27
25	0	616	LUT	C20-C13-C14	-3.28	118.33	122.92
26	A6	616	NEX	C40-C33-C34	-3.28	118.33	122.92
23	BV	605	CHL	C3B-C4B-NB	3.28	113.56	110.52
23	BU	606	CHL	CMB-C2B-C1B	3.28	130.36	125.37
23	0	605	CHL	C2D-C1D-ND	3.28	112.52	110.10
23	A2	605	CHL	C1D-ND-C4D	-3.28	104.01	106.33
23	g	609	CHL	CMD-C2D-C3D	-3.28	120.08	127.61
23	N	606	CHL	CMB-C2B-C1B	3.27	130.36	125.37
23	Y	308	CHL	CMB-C2B-C1B	3.27	130.36	125.37
24	BV	610	CLA	O2D-CGD-CBD	3.27	117.08	111.27
23	9	606	CHL	C1D-ND-C4D	-3.27	104.01	106.33
25	BV	614	LUT	C35-C15-C14	3.27	130.18	123.47
23	S	605	CHL	CMB-C2B-C1B	3.27	130.35	125.37
23	Y	306	CHL	CMB-C2B-C1B	3.27	130.35	125.37
23	5	609	CHL	CHD-C4C-C3C	-3.27	120.03	124.84
23	A6	601	CHL	C3B-C4B-NB	3.27	113.55	110.52
25	N	615	LUT	C20-C13-C14	-3.27	118.34	122.92
24	Aw	102	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
23	y	302	CHL	C3B-C4B-NB	3.27	113.55	110.52
34	Av	102	DGD	O3G-C3G-C2G	-3.27	103.01	110.90
23	BB	308	CHL	C1-C2-C3	-3.27	120.39	126.04
23	N	605	CHL	C1D-ND-C4D	-3.27	104.01	106.33
23	Au	607	CHL	C3D-C4D-ND	3.27	115.53	110.24
24	BD	407	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	0	606	CHL	CHB-C1B-NB	-3.27	120.80	124.26
26	BB	320	NEX	C20-C13-C14	-3.27	118.35	122.92
28	8	312	XAT	C39-C29-C28	-3.27	112.93	118.08
25	n	615	LUT	C15-C35-C34	3.27	130.17	123.47
23	s	601	CHL	C3D-C4D-ND	3.27	115.52	110.24
23	Ba	302	CHL	C3D-C4D-ND	3.27	115.52	110.24
23	n	601	CHL	C3D-C4D-ND	3.27	115.52	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A6	605	CHL	CMB-C2B-C1B	3.27	130.34	125.37
25	A2	615	LUT	C20-C13-C14	-3.27	118.35	122.92
23	6	605	CHL	C2D-C1D-ND	3.26	112.51	110.10
25	BU	615	LUT	C20-C13-C14	-3.26	118.35	122.92
23	n	607	CHL	C3D-C4D-ND	3.26	115.52	110.24
25	BB	317	LUT	C20-C13-C14	-3.26	118.35	122.92
23	n	608	CHL	C6-C5-C3	-3.26	109.28	114.62
29	v	617	BCR	C15-C16-C17	-3.26	116.79	123.47
23	BQ	605	CHL	CAC-C3C-C4C	3.26	129.04	124.81
23	N	607	CHL	C3D-C4D-ND	3.26	115.52	110.24
24	r	608	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
26	5	617	NEX	C12-C13-C14	3.26	123.94	118.94
23	5	608	CHL	CMB-C2B-C1B	3.26	130.34	125.37
23	A2	601	CHL	C1D-ND-C4D	-3.26	104.02	106.33
23	BV	605	CHL	CMD-C2D-C3D	-3.26	120.11	127.61
28	AB	312	XAT	C19-C9-C8	-3.26	112.94	118.08
26	s	616	NEX	C19-C9-C10	-3.26	118.36	122.92
23	Y	308	CHL	C1-C2-C3	-3.26	120.41	126.04
23	Ba	302	CHL	C3B-C4B-NB	3.26	113.54	110.52
28	AA	301	XAT	C10-C11-C12	-3.26	113.05	123.22
24	2	402	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	Au	609	CHL	C1D-ND-C4D	-3.26	104.02	106.33
23	AB	306	CHL	CAC-C3C-C4C	3.26	129.04	124.81
23	A6	601	CHL	C3D-C4D-ND	3.26	115.50	110.24
24	8	308	CLA	C2A-C3A-C4A	3.26	107.13	101.87
23	0	609	CHL	CHD-C4C-C3C	-3.25	120.06	124.84
26	A6	616	NEX	C12-C13-C14	3.25	123.93	118.94
23	BQ	607	CHL	C3D-C4D-ND	3.25	115.50	110.24
24	I	102	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
23	n	607	CHL	C1D-ND-C4D	-3.25	104.02	106.33
24	S	613	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
28	n	619	XAT	C39-C29-C28	-3.25	112.95	118.08
23	N	609	CHL	CAC-C3C-C4C	3.25	129.03	124.81
23	r	606	CHL	CMB-C2B-C1B	3.25	130.32	125.37
23	BJ	608	CHL	CHB-C1B-NB	-3.25	120.82	124.26
23	Au	605	CHL	C1D-ND-C4D	-3.25	104.03	106.33
23	A2	601	CHL	C3D-C4D-ND	3.25	115.50	110.24
23	A2	606	CHL	CMB-C2B-C1B	3.25	130.32	125.37
23	A6	606	CHL	C3D-C4D-ND	3.25	115.49	110.24
26	5	617	NEX	C19-C9-C10	-3.25	118.37	122.92
28	7	301	XAT	C10-C11-C12	-3.25	113.08	123.22
23	9	608	CHL	CMB-C2B-C1B	3.25	130.31	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	610	CLA	O2D-CGD-CBD	3.25	117.03	111.27
25	G	616	LUT	C20-C13-C14	-3.24	118.38	122.92
25	Au	616	LUT	C20-C13-C14	-3.24	118.38	122.92
23	y	308	CHL	C3D-C4D-ND	3.24	115.49	110.24
23	G	606	CHL	CAC-C3C-C4C	3.24	129.02	124.81
23	r	607	CHL	C1D-ND-C4D	-3.24	104.03	106.33
23	n	608	CHL	C2D-C1D-ND	3.24	112.49	110.10
24	BB	312	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
23	AA	309	CHL	C3D-C4D-ND	3.24	115.48	110.24
26	BB	318	NEX	C32-C33-C34	3.24	123.91	118.94
23	6	609	CHL	C6-C5-C3	-3.24	109.32	114.62
23	y	302	CHL	C3D-C4D-ND	3.24	115.48	110.24
23	Y	308	CHL	C4-C3-C5	3.24	120.72	115.27
25	AA	317	LUT	C20-C13-C14	-3.24	118.39	122.92
23	S	606	CHL	C3D-C4D-ND	3.24	115.47	110.24
23	BQ	601	CHL	C3D-C4D-ND	3.24	115.47	110.24
24	N	610	CLA	O2D-CGD-CBD	3.23	117.02	111.27
23	7	307	CHL	CAC-C3C-C4C	3.23	129.01	124.81
23	g	608	CHL	CHB-C1B-NB	-3.23	120.83	124.26
23	r	605	CHL	CHD-C4C-C3C	-3.23	120.09	124.84
23	6	608	CHL	C4A-NA-C1A	3.23	108.16	106.71
26	S	616	NEX	C12-C13-C14	3.23	123.90	118.94
24	6	610	CLA	CHB-C4A-NA	3.23	128.98	124.51
23	Au	606	CHL	CAC-C3C-C4C	3.23	129.00	124.81
25	r	615	LUT	C39-C29-C28	3.23	123.17	118.08
23	BQ	608	CHL	C6-C5-C3	-3.23	109.34	114.62
28	BB	301	XAT	C39-C29-C28	-3.23	112.99	118.08
23	Au	605	CHL	C3D-C4D-ND	3.23	115.46	110.24
25	BB	317	LUT	C15-C35-C34	3.23	130.09	123.47
23	8	307	CHL	C3D-C4D-ND	3.23	115.46	110.24
23	Ba	308	CHL	C3D-C4D-ND	3.23	115.46	110.24
25	9	616	LUT	C40-C33-C34	-3.23	118.41	122.92
23	9	606	CHL	C2D-C1D-ND	3.22	112.48	110.10
23	BU	605	CHL	C1-C2-C3	-3.22	120.47	126.04
23	A2	607	CHL	C3D-C4D-ND	3.22	115.45	110.24
32	l	102	SQD	O9-S-C6	3.22	110.77	106.94
23	S	601	CHL	C3D-C4D-ND	3.22	115.45	110.24
23	r	605	CHL	C2C-C3C-C4C	-3.22	104.19	106.49
23	7	309	CHL	C3D-C4D-ND	3.22	115.45	110.24
23	Au	601	CHL	CMB-C2B-C1B	3.22	130.27	125.37
23	BJ	606	CHL	CMB-C2B-C1B	3.22	130.27	125.37
26	Au	617	NEX	C28-C29-C30	3.22	123.88	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	r	606	CHL	C2D-C1D-ND	3.22	112.47	110.10
24	G	614	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
24	Au	614	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
23	Y	308	CHL	C3D-C4D-ND	3.22	115.44	110.24
24	c	506	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
23	9	605	CHL	CMB-C2B-C1B	3.21	130.26	125.37
23	G	605	CHL	C3D-C4D-ND	3.21	115.44	110.24
25	BU	615	LUT	C39-C29-C28	3.21	123.14	118.08
23	5	605	CHL	C2D-C1D-ND	3.21	112.47	110.10
23	Au	608	CHL	C2D-C1D-ND	3.21	112.47	110.10
24	Ba	313	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
23	6	607	CHL	C3D-C4D-ND	3.21	115.44	110.24
23	8	306	CHL	CAC-C3C-C4C	3.21	128.98	124.81
23	S	606	CHL	C1D-ND-C4D	-3.21	104.05	106.33
23	5	607	CHL	C3D-C4D-ND	3.21	115.44	110.24
28	BJ	619	XAT	C20-C13-C12	-3.21	113.02	118.08
23	7	306	CHL	CAC-C3C-C4C	3.21	128.98	124.81
24	0	602	CLA	C3B-C4B-NB	-3.21	107.53	110.52
23	s	606	CHL	C3D-C4D-ND	3.21	115.43	110.24
24	s	604	CLA	CHB-C1B-NB	3.21	127.66	124.26
23	5	605	CHL	CMB-C2B-C1B	3.21	130.26	125.37
23	Y	307	CHL	CMB-C2B-C1B	3.21	130.26	125.37
25	A2	616	LUT	C20-C13-C14	-3.21	118.43	122.92
23	y	309	CHL	C2D-C1D-ND	3.21	112.47	110.10
23	BB	308	CHL	C3D-C4D-ND	3.21	115.43	110.24
23	BQ	607	CHL	C3B-C4B-NB	3.21	113.49	110.52
28	BQ	619	XAT	C39-C29-C28	-3.21	113.02	118.08
28	A2	619	XAT	C39-C29-C28	-3.21	113.02	118.08
25	BJ	615	LUT	C20-C13-C14	-3.21	118.43	122.92
23	Y	306	CHL	C3B-C4B-NB	3.21	113.49	110.52
25	6	616	LUT	C15-C35-C34	3.21	130.04	123.47
23	Ba	309	CHL	CHD-C4C-C3C	-3.21	120.13	124.84
26	s	616	NEX	C12-C13-C14	3.21	123.86	118.94
25	r	615	LUT	C20-C13-C14	-3.21	118.43	122.92
23	5	601	CHL	C3D-C4D-ND	3.20	115.42	110.24
23	BU	605	CHL	C6-C5-C3	-3.20	109.38	114.62
26	BB	320	NEX	C32-C33-C34	3.20	123.86	118.94
23	6	606	CHL	CHB-C1B-NB	-3.20	120.86	124.26
23	0	607	CHL	C3D-C4D-ND	3.20	115.42	110.24
34	h	102	DGD	O6D-C1D-O3G	-3.20	102.39	109.97
31	BG	403	PL9	C7-C3-C2	-3.20	119.09	123.30
23	s	605	CHL	C3B-C4B-NB	3.20	113.49	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A6	606	CHL	C1D-ND-C4D	-3.20	104.06	106.33
25	6	616	LUT	C20-C13-C14	-3.20	118.44	122.92
24	y	313	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
26	N	617	NEX	C15-C35-C34	3.20	130.03	123.47
23	AA	308	CHL	CMB-C2B-C1B	3.20	130.24	125.37
28	Y	301	XAT	C39-C29-C28	-3.20	113.03	118.08
23	9	608	CHL	C3D-C4D-ND	3.20	115.42	110.24
23	7	302	CHL	CHC-C4B-NB	-3.20	120.87	124.26
23	N	605	CHL	C3D-C4D-ND	3.20	115.41	110.24
24	6	613	CLA	C1-C2-C3	-3.20	120.51	126.04
23	AA	307	CHL	CAC-C3C-C4C	3.20	128.96	124.81
31	d	403	PL9	C22-C23-C24	-3.20	119.96	127.66
23	A2	605	CHL	C3D-C4D-ND	3.20	115.41	110.24
23	BB	307	CHL	CMB-C2B-C1B	3.19	130.24	125.37
23	y	309	CHL	CHD-C4C-C3C	-3.19	120.14	124.84
25	BQ	615	LUT	C15-C35-C34	3.19	130.02	123.47
23	7	308	CHL	CMB-C2B-C1B	3.19	130.23	125.37
25	9	615	LUT	C40-C33-C34	-3.19	118.45	122.92
23	G	608	CHL	C2D-C1D-ND	3.19	112.46	110.10
23	BU	607	CHL	C1D-ND-C4D	-3.19	104.07	106.33
25	g	615	LUT	C20-C13-C14	-3.19	118.45	122.92
32	BO	102	SQD	O9-S-C6	3.19	110.73	106.94
29	h	101	BCR	C2-C1-C6	3.19	115.39	110.48
23	Au	607	CHL	C1-C2-C3	-3.19	120.53	126.04
23	0	601	CHL	C3D-C4D-ND	3.19	115.39	110.24
24	BQ	614	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
26	r	617	NEX	C32-C33-C34	3.19	123.83	118.94
24	BQ	610	CLA	C3B-C4B-NB	-3.19	107.56	110.52
24	b	611	CLA	CAC-C3C-C4C	-3.19	120.68	124.81
23	AA	306	CHL	CAC-C3C-C4C	3.19	128.94	124.81
25	BB	316	LUT	C20-C13-C14	-3.19	118.46	122.92
23	BU	606	CHL	C2D-C1D-ND	3.18	112.45	110.10
23	y	306	CHL	C3B-C4B-NB	3.18	113.47	110.52
28	BB	301	XAT	C40-C33-C32	-3.18	113.06	118.08
23	8	304	CHL	CAC-C3C-C4C	3.18	128.94	124.81
26	n	617	NEX	C12-C13-C14	3.18	123.82	118.94
23	0	607	CHL	CMB-C2B-C1B	3.18	130.22	125.37
23	BV	606	CHL	C3D-C4D-ND	3.18	115.38	110.24
23	r	605	CHL	C1-C2-C3	-3.18	120.54	126.04
28	N	619	XAT	C19-C9-C8	-3.18	113.06	118.08
23	g	606	CHL	CAC-C3C-C4C	3.18	128.94	124.81
24	A2	611	CLA	O2D-CGD-O1D	-3.18	117.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	606	CHL	CAC-C3C-C4C	3.18	128.94	124.81
24	AB	303	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	g	606	CHL	CMB-C2B-C1B	3.18	130.21	125.37
23	S	601	CHL	C3B-C4B-NB	3.18	113.46	110.52
23	AB	306	CHL	CHC-C4B-NB	-3.18	120.89	124.26
26	BV	616	NEX	C12-C13-C14	3.18	123.82	118.94
24	N	611	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
23	9	601	CHL	C3D-C4D-ND	3.18	115.38	110.24
26	y	318	NEX	C19-C9-C10	-3.18	118.47	122.92
23	A2	608	CHL	C2D-C1D-ND	3.18	112.44	110.10
23	A2	608	CHL	CMB-C2B-C1B	3.18	130.21	125.37
26	G	617	NEX	C28-C29-C30	3.18	123.81	118.94
24	n	614	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
25	n	616	LUT	C20-C13-C14	-3.18	118.47	122.92
23	AB	306	CHL	CMB-C2B-C1B	3.18	130.21	125.37
23	9	607	CHL	C3D-C4D-ND	3.18	115.37	110.24
23	A6	607	CHL	CMB-C2B-C1B	3.17	130.20	125.37
25	BQ	615	LUT	C40-C33-C34	-3.17	118.48	122.92
23	8	307	CHL	CMD-C2D-C3D	-3.17	120.31	127.61
23	Ba	306	CHL	C3B-C4B-NB	3.17	113.46	110.52
28	G	619	XAT	C10-C11-C12	-3.17	113.32	123.22
25	Y	317	LUT	C15-C35-C34	3.17	129.97	123.47
32	BO	102	SQD	O8-S-C6	3.17	110.79	105.74
23	G	609	CHL	CAC-C3C-C4C	3.17	128.92	124.81
23	7	310	CHL	C1-C2-C3	-3.17	120.56	126.04
23	0	608	CHL	C4A-NA-C1A	3.17	108.13	106.71
24	a	407	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
23	Ba	307	CHL	C3B-C4B-NB	3.17	113.45	110.52
23	N	608	CHL	C1-C2-C3	-3.17	120.56	126.04
28	Au	619	XAT	C10-C11-C12	-3.17	113.33	123.22
28	5	619	XAT	C40-C33-C32	-3.17	113.09	118.08
28	Ba	301	XAT	C39-C29-C28	-3.17	113.09	118.08
23	A2	608	CHL	C6-C5-C3	-3.17	109.44	114.62
24	5	612	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	N	616	LUT	C20-C13-C14	-3.17	118.49	122.92
23	A6	607	CHL	C2D-C1D-ND	3.16	112.44	110.10
24	BF	502	CLA	C3B-C4B-NB	-3.16	107.58	110.52
26	BQ	617	NEX	C12-C13-C14	3.16	123.79	118.94
23	BV	607	CHL	CHD-C4C-C3C	-3.16	120.19	124.84
29	BF	516	BCR	C15-C16-C17	-3.16	117.00	123.47
25	g	616	LUT	C20-C13-C14	-3.16	118.50	122.92
23	Au	608	CHL	C3D-C4D-ND	3.16	115.35	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	318	NEX	C32-C33-C34	3.16	123.79	118.94
24	v	614	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
23	BV	607	CHL	C3B-C4B-NB	3.16	113.44	110.52
23	N	608	CHL	CMB-C2B-C1B	3.16	130.18	125.37
23	5	606	CHL	CHB-C1B-NB	-3.16	120.92	124.26
25	8	311	LUT	C35-C15-C14	3.16	129.94	123.47
23	BV	606	CHL	O2D-CGD-O1D	-3.15	117.67	123.84
23	g	609	CHL	CAC-C3C-C4C	3.15	128.90	124.81
23	5	606	CHL	CAC-C3C-C4C	3.15	128.90	124.81
24	B	614	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	8	311	LUT	C20-C13-C14	-3.15	118.51	122.92
24	BD	406	CLA	CHD-C1D-ND	-3.15	121.56	124.45
23	BJ	607	CHL	CHB-C4A-NA	3.15	128.87	124.51
23	r	605	CHL	C1D-ND-C4D	-3.15	104.10	106.33
28	g	619	XAT	C20-C13-C12	-3.15	113.12	118.08
29	BE	618	BCR	C27-C26-C25	3.15	127.30	122.73
25	0	615	LUT	C15-C35-C34	3.15	129.92	123.47
32	l	102	SQD	O8-S-C6	3.15	110.76	105.74
26	A2	617	NEX	C32-C33-C34	3.15	123.77	118.94
23	Au	605	CHL	CMB-C2B-C1B	3.15	130.16	125.37
26	G	617	NEX	C32-C33-C34	3.15	123.77	118.94
23	0	609	CHL	C3B-C4B-NB	3.15	113.43	110.52
28	Y	301	XAT	C40-C33-C32	-3.15	113.12	118.08
23	g	607	CHL	CHB-C4A-NA	3.15	128.86	124.51
23	N	608	CHL	C6-C5-C3	-3.15	109.47	114.62
24	1	502	CLA	C3B-C4B-NB	-3.15	107.60	110.52
28	7	318	XAT	C40-C33-C32	-3.14	113.12	118.08
23	y	310	CHL	C1-C2-C3	-3.14	120.60	126.04
23	5	605	CHL	C3B-C4B-NB	3.14	113.43	110.52
23	Au	609	CHL	CMB-C2B-C1B	3.14	130.16	125.37
29	BK	101	BCR	C2-C1-C6	3.14	115.32	110.48
23	0	608	CHL	C3B-C4B-NB	3.14	113.43	110.52
26	7	319	NEX	C12-C13-C14	3.14	123.76	118.94
26	s	616	NEX	C32-C33-C34	3.14	123.76	118.94
23	AA	302	CHL	CHC-C4B-NB	-3.14	120.93	124.26
23	AB	304	CHL	CAC-C3C-C4C	3.14	128.89	124.81
23	y	310	CHL	CAC-C3C-C4C	3.14	128.89	124.81
23	N	608	CHL	C2D-C1D-ND	3.14	112.42	110.10
23	Ba	307	CHL	CMB-C2B-C1B	3.14	130.15	125.37
26	r	617	NEX	C12-C13-C14	3.14	123.76	118.94
24	BB	303	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
24	BE	616	CLA	O2D-CGD-O1D	-3.14	117.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	y	307	CHL	CMB-C2B-C1B	3.14	130.15	125.37
23	BQ	607	CHL	CMB-C2B-C1B	3.14	130.15	125.37
24	n	612	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	S	615	LUT	C1-C6-C7	3.14	124.66	115.78
23	6	601	CHL	C3D-C4D-ND	3.14	115.31	110.24
25	A6	615	LUT	C1-C6-C7	3.14	124.66	115.78
25	Y	316	LUT	C20-C13-C14	-3.14	118.53	122.92
23	0	608	CHL	CMB-C2B-C1B	3.14	130.15	125.37
28	y	301	XAT	C39-C29-C28	-3.14	113.13	118.08
24	8	303	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
28	BU	616	XAT	C39-C29-C28	-3.14	113.13	118.08
23	A2	601	CHL	C4-C3-C5	3.14	120.55	115.27
24	c	502	CLA	C3B-C4B-NB	-3.13	107.61	110.52
23	AB	306	CHL	C4A-NA-C1A	3.13	108.11	106.71
23	7	308	CHL	C4-C3-C5	3.13	120.54	115.27
23	n	607	CHL	CMB-C2B-C1B	3.13	130.14	125.37
23	9	606	CHL	CHB-C1B-NB	-3.13	120.94	124.26
23	s	606	CHL	O2D-CGD-O1D	-3.13	117.72	123.84
23	5	609	CHL	CMD-C2D-C3D	-3.13	120.41	127.61
26	g	617	NEX	C28-C29-C30	3.13	123.74	118.94
23	BJ	609	CHL	CAC-C3C-C4C	3.13	128.87	124.81
24	BQ	612	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	5	608	CHL	C3D-C4D-ND	3.13	115.30	110.24
26	BB	320	NEX	C12-C13-C14	3.13	123.74	118.94
23	A6	601	CHL	C1D-ND-C4D	-3.13	104.11	106.33
28	AA	318	XAT	C40-C33-C32	-3.13	113.15	118.08
24	B	603	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	Y	310	CHL	CMD-C2D-C3D	-3.13	120.42	127.61
26	N	617	NEX	C32-C33-C34	3.13	123.74	118.94
23	BB	302	CHL	CMB-C2B-C1B	3.13	130.13	125.37
25	0	616	LUT	C15-C35-C34	3.12	129.87	123.47
28	r	616	XAT	C39-C29-C28	-3.12	113.16	118.08
23	G	605	CHL	CMB-C2B-C1B	3.12	130.12	125.37
23	BJ	606	CHL	CAC-C3C-C4C	3.12	128.86	124.81
25	y	316	LUT	C35-C15-C14	3.12	129.87	123.47
23	AA	310	CHL	C1-C2-C3	-3.12	120.64	126.04
23	6	607	CHL	CMB-C2B-C1B	3.12	130.12	125.37
23	5	605	CHL	CAC-C3C-C4C	3.12	128.86	124.81
26	BJ	617	NEX	C28-C29-C30	3.12	123.73	118.94
23	6	605	CHL	C3B-C4B-NB	3.12	113.41	110.52
24	BU	601	CLA	C3B-C4B-NB	-3.12	107.62	110.52
23	r	613	CHL	CMD-C2D-C3D	-3.12	120.44	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BU	613	CHL	CMD-C2D-C3D	-3.12	120.44	127.61
26	Au	617	NEX	C32-C33-C34	3.12	123.72	118.94
23	5	608	CHL	C2D-C1D-ND	3.12	112.40	110.10
23	0	607	CHL	C1-C2-C3	-3.12	120.65	126.04
23	n	609	CHL	C3B-C4B-NB	3.12	113.41	110.52
23	6	605	CHL	C4A-NA-C1A	3.12	108.11	106.71
25	N	615	LUT	C40-C33-C34	-3.12	118.56	122.92
23	BB	307	CHL	CHB-C4A-NA	3.12	128.82	124.51
23	n	609	CHL	C2D-C1D-ND	3.11	112.40	110.10
23	G	601	CHL	CMB-C2B-C1B	3.11	130.11	125.37
23	n	607	CHL	C3B-C4B-NB	3.11	113.40	110.52
23	A2	608	CHL	C1-C2-C3	-3.11	120.66	126.04
25	y	316	LUT	C15-C35-C34	3.11	129.85	123.47
23	Au	608	CHL	C6-C5-C3	-3.11	109.53	114.62
26	AA	319	NEX	C12-C13-C14	3.11	123.71	118.94
24	5	610	CLA	C3B-C4B-NB	-3.11	107.63	110.52
23	G	609	CHL	CHD-C4C-C3C	-3.11	120.27	124.84
23	Au	608	CHL	CMB-C2B-C1B	3.11	130.10	125.37
26	Au	617	NEX	C12-C13-C14	3.11	123.71	118.94
23	g	607	CHL	CAC-C3C-C4C	3.11	128.84	124.81
25	5	616	LUT	C40-C33-C34	-3.11	118.57	122.92
24	BE	615	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
26	A2	617	NEX	C15-C35-C34	3.11	129.84	123.47
26	BV	616	NEX	C19-C9-C10	-3.11	118.57	122.92
28	n	619	XAT	C20-C13-C12	-3.11	113.18	118.08
23	0	608	CHL	C2D-C1D-ND	3.11	112.39	110.10
23	G	608	CHL	CMB-C2B-C1B	3.11	130.10	125.37
28	g	619	XAT	C40-C33-C32	-3.11	113.18	118.08
25	BV	615	LUT	C40-C33-C34	-3.11	118.57	122.92
23	Au	609	CHL	CHB-C4A-NA	3.11	128.81	124.51
23	8	306	CHL	CMB-C2B-C1B	3.11	130.10	125.37
23	A6	606	CHL	CMB-C2B-C1B	3.11	130.10	125.37
25	AB	311	LUT	C39-C29-C28	3.10	122.97	118.08
24	a	406	CLA	CHD-C1D-ND	-3.10	121.60	124.45
23	9	605	CHL	C3B-C4B-NB	3.10	113.39	110.52
26	n	617	NEX	C32-C33-C34	3.10	123.70	118.94
25	BJ	616	LUT	C8-C9-C10	3.10	123.70	118.94
25	BV	615	LUT	C15-C35-C34	3.10	129.83	123.47
25	y	317	LUT	C40-C33-C34	-3.10	118.58	122.92
23	N	607	CHL	C6-C5-C3	-3.10	109.55	114.62
24	BV	609	CLA	CHB-C4A-NA	3.10	128.80	124.51
23	AA	310	CHL	C4-C3-C5	3.10	120.49	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	G	607	CHL	C1-C2-C3	-3.10	120.68	126.04
23	AA	308	CHL	O2A-CGA-CBA	3.10	121.64	111.91
23	BU	606	CHL	O2A-CGA-CBA	3.10	121.64	111.91
23	8	306	CHL	CHC-C4B-NB	-3.10	120.97	124.26
24	r	601	CLA	C3B-C4B-NB	-3.10	107.64	110.52
28	Au	619	XAT	C19-C9-C8	-3.10	113.19	118.08
25	0	615	LUT	C35-C15-C14	3.10	129.82	123.47
23	AB	304	CHL	CMB-C2B-C1B	3.10	130.09	125.37
24	v	614	CLA	C1-C2-C3	-3.10	120.68	126.04
23	0	609	CHL	C6-C5-C3	-3.10	109.55	114.62
23	G	608	CHL	C3D-C4D-ND	3.10	115.25	110.24
23	s	607	CHL	CHD-C4C-C3C	-3.10	120.29	124.84
23	BJ	601	CHL	CHB-C1B-NB	-3.10	120.98	124.26
23	N	601	CHL	C4-C3-C5	3.10	120.48	115.27
23	BB	309	CHL	OMC-CMC-C2C	-3.10	118.69	125.69
23	0	605	CHL	C3B-C4B-NB	3.10	113.39	110.52
23	S	606	CHL	CMB-C2B-C1B	3.10	130.08	125.37
24	BF	507	CLA	C3B-C4B-NB	-3.09	107.64	110.52
28	G	619	XAT	C19-C9-C8	-3.09	113.20	118.08
28	y	301	XAT	C20-C13-C12	-3.09	113.20	118.08
23	BB	302	CHL	CHB-C1B-NB	-3.09	120.98	124.26
23	Y	307	CHL	CHB-C4A-NA	3.09	128.79	124.51
25	s	615	LUT	C15-C35-C34	3.09	129.81	123.47
26	BV	616	NEX	C32-C33-C34	3.09	123.69	118.94
23	0	606	CHL	CHB-C4A-NA	3.09	128.79	124.51
28	BJ	619	XAT	C40-C33-C32	-3.09	113.20	118.08
23	S	601	CHL	C1D-ND-C4D	-3.09	104.14	106.33
29	c	515	BCR	C15-C16-C17	-3.09	117.14	123.47
23	A6	606	CHL	O2D-CGD-O1D	-3.09	117.80	123.84
23	r	606	CHL	O2A-CGA-CBA	3.09	121.60	111.91
25	n	615	LUT	C40-C33-C34	-3.09	118.60	122.92
25	BV	614	LUT	C20-C13-C14	-3.09	118.60	122.92
23	6	606	CHL	CHB-C4A-NA	3.09	128.78	124.51
23	y	308	CHL	CMB-C2B-C1B	3.09	130.07	125.37
25	S	615	LUT	C19-C9-C8	3.09	122.94	118.08
33	4	102	HEM	C4D-ND-C1D	3.09	108.26	105.07
24	Y	303	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
26	BJ	617	NEX	C12-C13-C14	3.09	123.68	118.94
23	A2	609	CHL	C3D-C4D-ND	3.09	115.23	110.24
23	s	607	CHL	C3B-C4B-NB	3.09	113.38	110.52
28	Ba	301	XAT	C20-C13-C12	-3.09	113.22	118.08
23	n	609	CHL	C3D-C4D-ND	3.09	115.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Ba	316	LUT	C20-C13-C14	-3.08	118.60	122.92
23	6	608	CHL	CMB-C2B-C1B	3.08	130.06	125.37
26	g	617	NEX	C12-C13-C14	3.08	123.67	118.94
24	BB	312	CLA	C3B-C4B-NB	-3.08	107.66	110.52
23	7	310	CHL	CMB-C2B-C1B	3.08	130.06	125.37
25	A2	616	LUT	C40-C33-C34	-3.08	118.61	122.92
23	N	609	CHL	C3D-C4D-ND	3.08	115.22	110.24
23	BU	605	CHL	CHD-C4C-C3C	-3.08	120.31	124.84
25	A2	615	LUT	C40-C33-C34	-3.08	118.61	122.92
23	BQ	609	CHL	C2D-C1D-ND	3.08	112.37	110.10
23	A2	607	CHL	C4-C3-C5	3.08	120.45	115.27
23	Ba	308	CHL	CMB-C2B-C1B	3.08	130.06	125.37
23	Ba	309	CHL	CMB-C2B-C1B	3.08	130.06	125.37
23	AB	305	CHL	C3D-C4D-ND	3.08	115.22	110.24
23	9	605	CHL	CAC-C3C-C4C	3.08	128.80	124.81
23	Y	307	CHL	CHB-C1B-NB	-3.08	121.00	124.26
23	S	606	CHL	O2D-CGD-O1D	-3.08	117.82	123.84
28	Au	619	XAT	C39-C29-C28	-3.08	113.23	118.08
26	n	617	NEX	C19-C9-C10	-3.07	118.62	122.92
23	BB	307	CHL	CHB-C1B-NB	-3.07	121.00	124.26
23	BU	613	CHL	CMB-C2B-C1B	3.07	130.05	125.37
34	BK	102	DGD	O6D-C1D-O3G	-3.07	102.69	109.97
31	d	403	PL9	C40-C39-C41	3.07	120.44	115.27
23	0	606	CHL	C1D-ND-C4D	-3.07	104.15	106.33
23	BU	607	CHL	C3D-C4D-ND	3.07	115.21	110.24
23	r	607	CHL	C3D-C4D-ND	3.07	115.21	110.24
23	7	310	CHL	C4-C3-C5	3.07	120.44	115.27
24	C	502	CLA	C3B-C4B-NB	-3.07	107.67	110.52
23	A6	605	CHL	CHB-C1B-NB	-3.07	121.01	124.26
24	D	401	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	A2	607	CHL	C1-C2-C3	-3.07	120.73	126.04
23	8	304	CHL	CMB-C2B-C1B	3.07	130.04	125.37
23	A2	607	CHL	CMB-C2B-C1B	3.07	130.04	125.37
24	9	612	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
25	BJ	616	LUT	C20-C13-C14	-3.07	118.62	122.92
23	5	609	CHL	C1-C2-C3	-3.07	120.73	126.04
23	7	306	CHL	CHD-C4C-C3C	-3.07	120.33	124.84
24	B	603	CLA	C3B-C4B-NB	-3.07	107.67	110.52
23	8	305	CHL	C3D-C4D-ND	3.07	115.20	110.24
28	N	619	XAT	C39-C29-C28	-3.07	113.24	118.08
23	AA	310	CHL	CMB-C2B-C1B	3.07	130.04	125.37
25	Ba	317	LUT	C40-C33-C34	-3.07	118.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	9	608	CHL	C2D-C1D-ND	3.07	112.36	110.10
24	B	614	CLA	C1-C2-C3	-3.07	120.74	126.04
23	Y	309	CHL	C1D-ND-C4D	-3.07	104.16	106.33
23	BB	309	CHL	C1D-ND-C4D	-3.07	104.16	106.33
23	7	302	CHL	C2D-C1D-ND	3.07	112.36	110.10
26	Ba	318	NEX	C32-C33-C34	3.06	123.64	118.94
24	BU	604	CLA	CHB-C4A-NA	3.06	128.75	124.51
26	y	318	NEX	C32-C33-C34	3.06	123.64	118.94
32	BG	406	SQD	O8-S-C6	3.06	110.62	105.74
28	BQ	619	XAT	C12-C13-C14	-3.06	114.24	118.94
24	v	606	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
28	Ba	301	XAT	C40-C33-C32	-3.06	113.25	118.08
23	AA	306	CHL	CHD-C4C-C3C	-3.06	120.34	124.84
23	N	608	CHL	C4A-NA-C1A	3.06	108.08	106.71
25	Ba	317	LUT	C20-C13-C14	-3.06	118.64	122.92
25	5	615	LUT	C12-C13-C14	3.06	123.63	118.94
23	6	608	CHL	C3B-C4B-NB	3.06	113.35	110.52
32	L	101	SQD	O8-S-C6	3.06	110.61	105.74
25	5	616	LUT	C8-C9-C10	3.06	123.63	118.94
23	6	607	CHL	C1-C2-C3	-3.06	120.76	126.04
25	N	616	LUT	C40-C33-C34	-3.06	118.64	122.92
28	G	619	XAT	C39-C29-C28	-3.06	113.26	118.08
23	9	609	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
28	BB	301	XAT	C19-C9-C8	-3.05	113.26	118.08
23	AA	307	CHL	CMB-C2B-C1B	3.05	130.02	125.37
23	7	307	CHL	CMB-C2B-C1B	3.05	130.02	125.37
23	y	307	CHL	C3B-C4B-NB	3.05	113.35	110.52
23	Ba	310	CHL	C1-C2-C3	-3.05	120.76	126.04
26	BJ	617	NEX	C32-C33-C34	3.05	123.63	118.94
24	BV	613	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	R	405	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	s	615	LUT	C40-C33-C34	-3.05	118.65	122.92
25	A6	615	LUT	C19-C9-C8	3.05	122.89	118.08
23	N	607	CHL	CMB-C2B-C1B	3.05	130.02	125.37
23	0	607	CHL	C2D-C1D-ND	3.05	112.35	110.10
26	g	617	NEX	C32-C33-C34	3.05	123.62	118.94
23	9	607	CHL	C6-C5-C3	-3.05	109.63	114.62
24	BQ	610	CLA	CMA-C3A-C2A	-3.05	101.52	113.83
24	A2	612	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	Y	312	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
25	s	614	LUT	C20-C13-C14	-3.05	118.65	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AA	317	LUT	C40-C33-C34	-3.05	118.65	122.92
24	BF	511	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
28	BJ	619	XAT	C39-C29-C28	-3.05	113.28	118.08
23	Au	601	CHL	CHB-C4A-NA	3.05	128.73	124.51
24	A	406	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	y	317	LUT	C20-C13-C14	-3.05	118.66	122.92
23	n	609	CHL	C1C-C2C-C3C	-3.05	104.70	107.11
23	n	609	CHL	CMD-C2D-C3D	-3.05	120.61	127.61
23	g	601	CHL	CHB-C1B-NB	-3.05	121.03	124.26
32	d	406	SQD	O8-S-C6	3.05	110.59	105.74
24	Y	313	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	n	607	CHL	C4-C3-C5	3.04	120.39	115.27
23	AA	310	CHL	CHC-C4B-NB	-3.04	121.03	124.26
23	r	613	CHL	CMB-C2B-C1B	3.04	130.00	125.37
24	N	612	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	G	608	CHL	C6-C5-C3	-3.04	109.64	114.62
26	G	617	NEX	C12-C13-C14	3.04	123.61	118.94
29	h	101	BCR	C11-C10-C9	-3.04	122.97	127.31
23	BQ	606	CHL	O2A-CGA-CBA	3.04	121.46	111.91
26	S	616	NEX	C32-C33-C34	3.04	123.61	118.94
23	S	605	CHL	CHB-C1B-NB	-3.04	121.04	124.26
23	G	608	CHL	O2A-CGA-CBA	3.04	121.45	111.91
23	e	601	CHL	CHB-C1B-NB	-3.04	121.04	124.26
25	y	316	LUT	C40-C33-C34	-3.04	118.66	122.92
23	5	607	CHL	C2D-C1D-ND	3.04	112.34	110.10
28	AA	318	XAT	C19-C9-C8	-3.04	113.29	118.08
28	A2	619	XAT	C19-C9-C8	-3.04	113.29	118.08
26	N	617	NEX	C19-C9-C10	-3.04	118.66	122.92
28	y	301	XAT	C40-C33-C32	-3.04	113.29	118.08
23	y	309	CHL	CMB-C2B-C1B	3.04	130.00	125.37
25	BV	614	LUT	C15-C35-C34	3.04	129.69	123.47
25	r	615	LUT	C7-C8-C9	-3.04	121.65	126.23
24	N	610	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	v	603	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	Au	608	CHL	O2A-CGA-CBA	3.04	121.44	111.91
23	S	607	CHL	C1D-ND-C4D	-3.03	104.18	106.33
25	Ba	316	LUT	C40-C33-C34	-3.03	118.67	122.92
24	BF	512	CLA	O2D-CGD-CBD	3.03	116.66	111.27
31	BG	403	PL9	C40-C39-C41	3.03	120.38	115.27
24	c	511	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
25	n	615	LUT	C20-C13-C14	-3.03	118.67	122.92
23	0	605	CHL	C4A-NA-C1A	3.03	108.07	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Y	302	CHL	CMB-C2B-C1B	3.03	129.99	125.37
23	6	608	CHL	C2D-C1D-ND	3.03	112.34	110.10
23	A2	601	CHL	CMB-C2B-C1B	3.03	129.99	125.37
24	R	405	CLA	CHD-C1D-ND	-3.03	121.67	124.45
23	n	608	CHL	CMB-C2B-C1B	3.03	129.99	125.37
23	BU	605	CHL	C1D-ND-C4D	-3.03	104.18	106.33
23	Y	306	CHL	CAC-C3C-C4C	3.03	128.74	124.81
24	Au	602	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	N	601	CHL	CMB-C2B-C1B	3.03	129.99	125.37
33	F	102	HEM	C4D-ND-C1D	3.03	108.20	105.07
26	BB	320	NEX	C19-C9-C10	-3.03	118.68	122.92
23	BJ	606	CHL	O2A-CGA-CBA	3.03	121.42	111.91
23	AA	309	CHL	OMC-CMC-C2C	-3.03	118.83	125.69
24	1	512	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
28	g	619	XAT	C39-C29-C28	-3.03	113.30	118.08
23	AB	307	CHL	C3D-C4D-ND	3.03	115.14	110.24
23	n	609	CHL	CAC-C3C-C4C	3.03	128.74	124.81
24	7	305	CLA	C3B-C4B-NB	-3.03	107.70	110.52
24	1	503	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	v	617	BCR	C15-C14-C13	-3.03	122.99	127.31
25	BB	316	LUT	C40-C33-C34	-3.03	118.68	122.92
23	Y	309	CHL	C3D-C4D-ND	3.03	115.14	110.24
26	BQ	617	NEX	C32-C33-C34	3.03	123.59	118.94
23	BQ	608	CHL	CMB-C2B-C1B	3.03	129.98	125.37
23	9	608	CHL	CMD-C2D-C3D	-3.03	120.65	127.61
23	BQ	607	CHL	C4-C3-C5	3.03	120.36	115.27
25	Y	316	LUT	C40-C33-C34	-3.03	118.68	122.92
28	7	318	XAT	C19-C9-C8	-3.03	113.31	118.08
29	K	102	BCR	C15-C16-C17	-3.03	117.28	123.47
23	5	609	CHL	CHC-C4B-NB	-3.03	121.05	124.26
25	0	615	LUT	C20-C13-C14	-3.03	118.69	122.92
25	BJ	615	LUT	C40-C33-C34	-3.02	118.69	122.92
23	BB	309	CHL	C3D-C4D-ND	3.02	115.13	110.24
23	n	605	CHL	C3D-C4D-ND	3.02	115.12	110.24
23	BB	310	CHL	C3D-C4D-ND	3.02	115.12	110.24
23	AB	307	CHL	CAC-C3C-C4C	3.02	128.73	124.81
24	G	602	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	5	603	CLA	C3B-C4B-NB	-3.02	107.72	110.52
24	A2	602	CLA	C3B-C4B-NB	-3.02	107.72	110.52
26	Ba	318	NEX	C19-C9-C10	-3.02	118.70	122.92
24	R	406	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	5	607	CHL	C6-C5-C3	-3.02	109.69	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	617	BCR	C15-C14-C13	-3.02	123.01	127.31
23	BQ	609	CHL	CMD-C2D-C3D	-3.02	120.68	127.61
23	6	601	CHL	C1-C2-C3	-3.01	120.83	126.04
24	B	601	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
24	s	609	CLA	CHB-C4A-NA	3.01	128.68	124.51
24	BB	313	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	A6	613	CLA	C3B-C4B-NB	-3.01	107.72	110.52
32	D	406	SQD	O8-S-C6	3.01	110.54	105.74
24	b	616	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	9	616	LUT	C20-C13-C14	-3.01	118.71	122.92
25	BV	615	LUT	C20-C13-C14	-3.01	118.71	122.92
23	8	304	CHL	C3B-C4B-NB	3.01	113.31	110.52
24	Au	612	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	N	607	CHL	C4-C3-C5	3.01	120.33	115.27
24	r	604	CLA	CHB-C4A-NA	3.01	128.67	124.51
23	BH	601	CHL	CHB-C1B-NB	-3.01	121.07	124.26
25	5	615	LUT	C40-C33-C34	-3.01	118.71	122.92
25	g	615	LUT	C40-C33-C34	-3.01	118.71	122.92
23	AB	307	CHL	C3B-C4B-NB	3.01	113.30	110.52
28	A2	619	XAT	C40-C33-C32	-3.01	113.34	118.08
23	Y	309	CHL	OMC-CMC-C2C	-3.01	118.89	125.69
24	Y	312	CLA	C3B-C4B-NB	-3.01	107.73	110.52
24	A	407	CLA	O2D-CGD-CBD	3.00	116.61	111.27
24	g	611	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
24	BV	604	CLA	C1-C2-C3	-3.00	121.89	126.75
23	BJ	601	CHL	CHB-C4A-NA	3.00	128.66	124.51
23	A2	609	CHL	C2D-C1D-ND	3.00	112.32	110.10
23	5	608	CHL	CMD-C2D-C3D	-3.00	120.71	127.61
23	Y	310	CHL	C3D-C4D-ND	3.00	115.09	110.24
23	g	606	CHL	O2A-CGA-CBA	3.00	121.33	111.91
25	G	616	LUT	C40-C33-C34	-3.00	118.72	122.92
23	g	601	CHL	CHB-C4A-NA	3.00	128.66	124.51
23	BB	302	CHL	CHB-C4A-NA	3.00	128.66	124.51
23	Y	308	CHL	CHB-C4A-NA	3.00	128.66	124.51
23	AA	302	CHL	C2D-C1D-ND	3.00	112.31	110.10
24	BB	305	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	BB	310	CHL	C2D-C1D-ND	3.00	112.31	110.10
24	b	610	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
24	S	610	CLA	C3B-C4B-NB	-3.00	107.73	110.52
25	5	615	LUT	C8-C9-C10	3.00	123.54	118.94
31	2	404	PL9	C7-C3-C2	-3.00	119.36	123.30
23	BQ	609	CHL	C1-C2-C3	-3.00	120.86	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	305	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	y	306	CHL	C3D-C4D-ND	3.00	115.08	110.24
23	BB	306	CHL	CAC-C3C-C4C	3.00	128.70	124.81
24	AA	313	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	Y	307	CHL	C3D-C4D-ND	3.00	115.08	110.24
24	s	609	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
24	BJ	611	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
26	A6	616	NEX	C32-C33-C34	3.00	123.54	118.94
23	8	307	CHL	C2D-C1D-ND	2.99	112.31	110.10
24	n	610	CLA	CMA-C3A-C2A	-2.99	101.75	113.83
23	Ba	308	CHL	CHB-C4A-NA	2.99	128.65	124.51
23	g	605	CHL	CAC-C3C-C4C	2.99	128.69	124.81
24	9	614	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
23	6	606	CHL	C1D-ND-C4D	-2.99	104.21	106.33
24	0	610	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
28	N	619	XAT	C40-C33-C32	-2.99	113.36	118.08
24	8	302	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	BQ	615	LUT	C20-C13-C14	-2.99	118.73	122.92
24	N	602	CLA	C3B-C4B-NB	-2.99	107.74	110.52
38	BD	408	PHO	O2D-CGD-O1D	-2.99	117.99	123.84
24	b	615	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	A2	616	LUT	C15-C35-C34	2.99	129.60	123.47
25	BQ	616	LUT	C20-C13-C14	-2.99	118.73	122.92
23	BU	607	CHL	CHB-C4A-NA	2.99	128.65	124.51
23	BB	308	CHL	CHB-C4A-NA	2.99	128.65	124.51
23	A6	606	CHL	C6-C5-C3	-2.99	109.73	114.62
23	Y	302	CHL	CHB-C1B-NB	-2.99	121.09	124.26
24	Ba	305	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
29	z	101	BCR	C33-C5-C6	-2.99	121.17	124.53
23	g	609	CHL	C1-C2-C3	-2.99	120.87	126.04
24	b	607	CLA	C3B-C4B-NB	-2.99	107.74	110.52
24	v	606	CLA	C3B-C4B-NB	-2.99	107.74	110.52
23	Ba	306	CHL	C3D-C4D-ND	2.99	115.07	110.24
23	AB	304	CHL	C2D-C1D-ND	2.99	112.31	110.10
23	BQ	601	CHL	C4-C3-C5	2.99	120.30	115.27
23	Ba	309	CHL	C2D-C1D-ND	2.99	112.31	110.10
23	A2	607	CHL	C6-C5-C3	-2.99	109.74	114.62
23	7	309	CHL	OMC-CMC-C2C	-2.99	118.94	125.69
24	BV	602	CLA	CHB-C4A-NA	2.98	128.64	124.51
24	Ba	315	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
23	9	601	CHL	CMB-C2B-C1B	2.98	129.91	125.37
24	A	406	CLA	O2D-CGD-O1D	-2.98	118.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	305	CLA	C3B-C4B-NB	-2.98	107.75	110.52
24	N	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	BJ	607	CHL	CAC-C3C-C4C	2.98	128.68	124.81
24	A2	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	BQ	605	CHL	C3D-C4D-ND	2.98	115.06	110.24
23	n	609	CHL	C1-C2-C3	-2.98	120.89	126.04
28	Y	301	XAT	C19-C9-C8	-2.98	113.38	118.08
24	c	505	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	BE	607	CLA	C3B-C4B-NB	-2.98	107.75	110.52
25	AA	316	LUT	C40-C33-C34	-2.98	118.75	122.92
24	v	601	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	Ba	302	CHL	C1D-ND-C4D	-2.98	104.22	106.33
24	A6	610	CLA	C3B-C4B-NB	-2.98	107.75	110.52
23	6	609	CHL	CMB-C2B-C1B	2.98	129.91	125.37
24	n	611	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
24	s	603	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
23	BV	606	CHL	CHB-C4A-NA	2.98	128.63	124.51
23	BB	310	CHL	CMB-C2B-C1B	2.98	129.90	125.37
31	D	403	PL9	C7-C8-C9	-2.98	121.84	126.79
24	AB	308	CLA	CHB-C4A-NA	2.98	128.63	124.51
24	B	606	CLA	C3B-C4B-NB	-2.98	107.75	110.52
23	BU	606	CHL	C4-C3-C5	2.97	120.28	115.27
23	BB	302	CHL	O2A-CGA-CBA	2.97	121.24	111.91
23	0	609	CHL	CMB-C2B-C1B	2.97	129.90	125.37
23	BB	307	CHL	C3D-C4D-ND	2.97	115.05	110.24
24	C	512	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
25	n	616	LUT	C40-C33-C34	-2.97	118.76	122.92
25	A6	614	LUT	C20-C13-C14	-2.97	118.76	122.92
24	1	506	CLA	C3B-C4B-NB	-2.97	107.76	110.52
23	BB	310	CHL	CMD-C2D-C3D	-2.97	120.77	127.61
23	6	607	CHL	C6-C5-C3	-2.97	109.76	114.62
25	AB	311	LUT	C12-C13-C14	2.97	123.50	118.94
26	5	617	NEX	C28-C29-C30	2.97	123.50	118.94
24	A2	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	n	610	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	BB	302	CHL	C6-C5-C3	-2.97	109.76	114.62
23	AB	304	CHL	C3B-C4B-NB	2.97	113.27	110.52
24	A6	612	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	6	608	CHL	CMD-C2D-C3D	-2.97	120.78	127.61
23	y	308	CHL	CHB-C4A-NA	2.97	128.62	124.51
24	5	602	CLA	C3B-C4B-NB	-2.97	107.76	110.52
24	s	602	CLA	CHB-C4A-NA	2.97	128.62	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	0	615	LUT	C40-C33-C34	-2.97	118.76	122.92
24	c	507	CLA	C3B-C4B-NB	-2.97	107.76	110.52
38	BD	408	PHO	O1D-CGD-CBD	2.97	129.68	124.74
24	BQ	611	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	s	606	CHL	CHB-C4A-NA	2.97	128.62	124.51
24	6	611	CLA	CHB-C4A-NA	2.97	128.62	124.51
25	A6	615	LUT	C40-C33-C34	-2.97	118.77	122.92
24	7	313	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	S	612	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
23	5	601	CHL	CMB-C2B-C1B	2.97	129.89	125.37
25	s	615	LUT	C20-C13-C14	-2.97	118.77	122.92
34	1	518	DGD	O5D-C6D-C5D	-2.97	103.56	109.05
24	s	613	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
25	Au	615	LUT	C12-C13-C14	2.97	123.49	118.94
23	A2	601	CHL	CMD-C2D-C3D	-2.96	120.79	127.61
24	N	614	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
24	BF	503	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
23	S	606	CHL	C6-C5-C3	-2.96	109.77	114.62
24	s	612	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	AB	302	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	n	606	CHL	O2A-CGA-CBA	2.96	121.20	111.91
29	B	617	BCR	C29-C30-C25	2.96	115.04	110.48
23	7	302	CHL	C3D-C4D-ND	2.96	115.03	110.24
23	BJ	609	CHL	C1-C2-C3	-2.96	120.92	126.04
24	S	613	CLA	C3B-C4B-NB	-2.96	107.77	110.52
24	BE	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	BV	612	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	Y	302	CHL	CHB-C4A-NA	2.96	128.60	124.51
24	BV	603	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	n	608	CHL	C1-C2-C3	-2.96	120.93	126.04
23	N	609	CHL	C2D-C1D-ND	2.96	112.28	110.10
24	B	609	CLA	C3B-C4B-NB	-2.96	107.77	110.52
26	9	617	NEX	C28-C29-C30	2.96	123.48	118.94
23	AB	304	CHL	C4A-NA-C1A	2.96	108.03	106.71
28	8	312	XAT	C5-C4-C3	-2.96	106.90	112.75
23	G	608	CHL	CMD-C2D-C3D	-2.96	120.81	127.61
25	Au	616	LUT	C40-C33-C34	-2.96	118.78	122.92
24	1	513	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	9	605	CHL	C3D-C4D-ND	2.96	115.02	110.24
23	N	607	CHL	C1-C2-C3	-2.95	120.93	126.04
23	Y	302	CHL	C6-C5-C3	-2.95	109.79	114.62
23	n	601	CHL	C4-C3-C5	2.95	120.24	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	408	SQD	C45-O47-C7	-2.95	110.52	117.79
25	N	616	LUT	C15-C35-C34	2.95	129.52	123.47
23	0	607	CHL	C6-C5-C3	-2.95	109.79	114.62
29	BE	618	BCR	C33-C5-C6	-2.95	121.21	124.53
24	b	613	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	G	609	CHL	C3D-C4D-ND	2.95	115.01	110.24
23	BU	605	CHL	CMD-C2D-C3D	-2.95	120.83	127.61
24	BF	502	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	6	605	CHL	C3D-C4D-ND	2.95	115.01	110.24
23	BU	605	CHL	O2A-CGA-CBA	2.95	121.16	111.91
25	G	615	LUT	C39-C29-C28	2.95	122.72	118.08
23	BQ	609	CHL	C3D-C4D-ND	2.95	115.01	110.24
24	Ba	312	CLA	C3B-C4B-NB	-2.95	107.78	110.52
24	A6	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	s	604	CLA	C1-C2-C3	-2.95	121.98	126.75
28	AA	301	XAT	C19-C9-C8	-2.95	113.43	118.08
24	BE	613	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
23	AB	306	CHL	C2D-C1D-ND	2.95	112.28	110.10
23	G	609	CHL	C4A-NA-C1A	2.94	108.03	106.71
24	C	511	CLA	C4A-NA-C1A	2.94	108.03	106.71
25	BJ	615	LUT	C39-C29-C28	2.94	122.72	118.08
23	A2	601	CHL	C1-C2-C3	-2.94	120.95	126.04
23	S	607	CHL	C3D-C4D-ND	2.94	115.00	110.24
23	Y	309	CHL	CMB-C2B-C1B	2.94	129.85	125.37
23	BB	306	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
23	BB	306	CHL	C3D-C4D-ND	2.94	115.00	110.24
32	BO	101	SQD	O8-S-C6	2.94	110.43	105.74
29	C	514	BCR	C33-C5-C6	-2.94	121.22	124.53
25	6	616	LUT	C32-C33-C34	2.94	123.45	118.94
24	c	509	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	r	615	LUT	C15-C35-C34	2.94	129.50	123.47
25	S	614	LUT	C20-C13-C14	-2.94	118.80	122.92
25	S	614	LUT	C40-C33-C34	-2.94	118.80	122.92
25	BU	615	LUT	C40-C33-C34	-2.94	118.80	122.92
23	y	307	CHL	O2A-CGA-CBA	2.94	121.14	111.91
32	2	408	SQD	O8-S-C6	2.94	110.43	105.74
38	R	407	PHO	O2D-CGD-O1D	-2.94	118.09	123.84
25	0	616	LUT	C12-C13-C14	2.94	123.45	118.94
23	7	306	CHL	CMB-C2B-C1B	2.94	129.85	125.37
29	BF	515	BCR	C33-C5-C6	-2.94	121.23	124.53
25	Au	615	LUT	C39-C29-C28	2.94	122.71	118.08
24	y	315	CLA	O2D-CGD-O1D	-2.94	118.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BU	601	CLA	CHB-C4A-NA	2.94	128.57	124.51
24	BJ	614	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
29	v	617	BCR	C33-C5-C6	-2.94	121.23	124.53
23	n	601	CHL	C1D-ND-C4D	-2.94	104.25	106.33
24	0	611	CLA	CHB-C4A-NA	2.94	128.57	124.51
23	AA	302	CHL	C3D-C4D-ND	2.94	114.99	110.24
23	8	306	CHL	C2D-C1D-ND	2.94	112.27	110.10
23	BQ	609	CHL	C3B-C4B-NB	2.94	113.24	110.52
24	5	612	CLA	C3B-C4B-NB	-2.94	107.79	110.52
24	v	610	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
23	5	601	CHL	CHB-C4A-NA	2.93	128.57	124.51
23	y	309	CHL	CMD-C2D-C3D	-2.93	120.86	127.61
24	9	603	CLA	C3B-C4B-NB	-2.93	107.79	110.52
24	0	614	CLA	C3B-C4B-NB	-2.93	107.79	110.52
24	BV	613	CLA	C3B-C4B-NB	-2.93	107.79	110.52
23	g	607	CHL	CMB-C2B-C1B	2.93	129.84	125.37
28	5	619	XAT	C39-C29-C28	-2.93	113.45	118.08
25	0	616	LUT	C32-C33-C34	2.93	123.44	118.94
23	BQ	608	CHL	C1-C2-C3	-2.93	120.97	126.04
23	r	605	CHL	O2A-CGA-CBA	2.93	121.11	111.91
23	Ba	308	CHL	C4-C3-C5	2.93	120.20	115.27
23	Y	310	CHL	C2D-C1D-ND	2.93	112.27	110.10
28	AA	318	XAT	C39-C29-C28	-2.93	113.46	118.08
23	BQ	601	CHL	C1D-ND-C4D	-2.93	104.25	106.33
23	Y	310	CHL	CMB-C2B-C1B	2.93	129.83	125.37
24	y	305	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	BQ	610	CLA	CHB-C4A-NA	2.93	128.56	124.51
24	5	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	C	503	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
38	a	408	PHO	O2D-CGD-O1D	-2.93	118.11	123.84
24	G	610	CLA	C3B-C4B-NB	-2.93	107.80	110.52
23	r	607	CHL	CHB-C4A-NA	2.93	128.56	124.51
34	H	102	DGD	O6D-C1D-O3G	-2.93	103.04	109.97
24	B	612	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
24	6	604	CLA	C3B-C4B-NB	-2.93	107.80	110.52
23	BJ	605	CHL	CAC-C3C-C4C	2.93	128.61	124.81
23	9	607	CHL	O2D-CGD-O1D	-2.93	118.12	123.84
24	B	610	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
24	C	506	CLA	C3B-C4B-NB	-2.93	107.80	110.52
28	9	619	XAT	C39-C29-C28	-2.93	113.47	118.08
29	b	618	BCR	C27-C26-C25	2.93	126.98	122.73
23	7	306	CHL	CMD-C2D-C3D	-2.93	120.89	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	603	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
23	AA	306	CHL	CMD-C2D-C3D	-2.92	120.89	127.61
23	5	606	CHL	CHB-C4A-NA	2.92	128.56	124.51
29	Ay	102	BCR	C15-C16-C17	-2.92	117.48	123.47
24	BF	509	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
25	7	316	LUT	C20-C13-C14	-2.92	118.83	122.92
24	c	504	CLA	C3B-C4B-NB	-2.92	107.80	110.52
25	A6	614	LUT	C40-C33-C34	-2.92	118.83	122.92
23	5	605	CHL	C3D-C4D-ND	2.92	114.97	110.24
23	AA	306	CHL	CMB-C2B-C1B	2.92	129.82	125.37
23	Au	608	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
23	N	601	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
25	S	614	LUT	C35-C15-C14	2.92	129.45	123.47
32	l	101	SQD	O8-S-C6	2.92	110.39	105.74
23	Y	306	CHL	C3D-C4D-ND	2.92	114.96	110.24
24	6	614	CLA	C3B-C4B-NB	-2.92	107.81	110.52
24	7	311	CLA	C3B-C4B-NB	-2.92	107.81	110.52
23	7	309	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
25	s	614	LUT	C15-C35-C34	2.92	129.45	123.47
23	r	606	CHL	C4-C3-C5	2.92	120.18	115.27
28	7	301	XAT	C19-C9-C8	-2.92	113.48	118.08
24	BE	604	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
34	Av	102	DGD	O6D-C1D-O3G	-2.92	103.07	109.97
23	8	304	CHL	C2D-C1D-ND	2.92	112.25	110.10
29	BK	101	BCR	C11-C10-C9	-2.92	123.15	127.31
29	v	617	BCR	C29-C30-C25	2.92	114.97	110.48
24	r	601	CLA	CHB-C4A-NA	2.92	128.54	124.51
24	b	608	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	BF	504	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	BJ	607	CHL	CMB-C2B-C1B	2.91	129.81	125.37
24	g	614	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	s	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	9	614	CLA	C3B-C4B-NB	-2.91	107.81	110.52
24	C	509	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	9	601	CHL	CHB-C4A-NA	2.91	128.54	124.51
23	G	609	CHL	CMB-C2B-C1B	2.91	129.80	125.37
23	0	605	CHL	C3D-C4D-ND	2.91	114.95	110.24
32	BD	412	SQD	O8-S-C6	2.91	110.38	105.74
24	y	311	CLA	C3B-C4B-NB	-2.91	107.81	110.52
23	0	601	CHL	C3B-C4B-NB	2.91	113.22	110.52
23	AA	306	CHL	C3B-C4B-NB	2.91	113.22	110.52
28	7	318	XAT	C39-C29-C28	-2.91	113.49	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	605	CHL	CMD-C2D-C3D	-2.91	120.92	127.61
34	C	518	DGD	O5D-C6D-C5D	-2.91	103.66	109.05
24	8	310	CLA	CHB-C4A-NA	2.91	128.54	124.51
25	g	616	LUT	C40-C33-C34	-2.91	118.85	122.92
23	N	608	CHL	C4-C3-C5	2.91	120.17	115.27
24	v	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
28	n	619	XAT	C40-C33-C32	-2.91	113.49	118.08
25	9	615	LUT	C8-C9-C10	2.91	123.41	118.94
29	Bb	101	BCR	C15-C16-C17	-2.91	117.51	123.47
24	C	513	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	A2	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	a	407	CLA	C3B-C4B-NB	-2.91	107.82	110.52
24	AA	312	CLA	C3B-C4B-NB	-2.91	107.82	110.52
28	G	619	XAT	C40-C33-C32	-2.91	113.50	118.08
23	AA	309	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
23	n	608	CHL	C4-C3-C5	2.91	120.16	115.27
23	G	601	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
28	7	301	XAT	C12-C13-C14	-2.91	114.48	118.94
23	5	607	CHL	C1C-C2C-C3C	-2.91	104.81	107.11
23	Au	601	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
24	y	312	CLA	C3B-C4B-NB	-2.91	107.82	110.52
23	G	606	CHL	O2A-CGA-CBA	2.90	121.02	111.91
23	Ba	307	CHL	O2A-CGA-CBA	2.90	121.02	111.91
24	b	604	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	AA	316	LUT	C20-C13-C14	-2.90	118.86	122.92
24	9	612	CLA	C3B-C4B-NB	-2.90	107.82	110.52
23	7	310	CHL	CHC-C4B-NB	-2.90	121.18	124.26
24	BE	603	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	n	606	CHL	C3B-C4B-NB	2.90	113.21	110.52
23	BV	605	CHL	CMB-C2B-C1B	2.90	129.79	125.37
24	v	613	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	A2	608	CHL	C4A-NA-C1A	2.90	108.01	106.71
23	BV	601	CHL	C1D-ND-C4D	-2.90	104.27	106.33
24	BV	604	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	G	615	LUT	C12-C13-C14	2.90	123.39	118.94
24	A2	614	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
38	a	408	PHO	O1D-CGD-CBD	2.90	129.57	124.74
23	g	607	CHL	CHB-C1B-NB	-2.90	121.19	124.26
24	Au	610	CLA	C1-C2-C3	-2.90	121.03	126.04
23	Au	606	CHL	O2A-CGA-CBA	2.90	121.01	111.91
24	v	604	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	B	602	CLA	O2D-CGD-O1D	-2.90	118.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	v	612	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	BF	509	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	BE	608	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	BJ	609	CHL	C3D-C4D-ND	2.90	114.93	110.24
25	g	615	LUT	C39-C29-C28	2.90	122.64	118.08
24	v	608	CLA	C3B-C4B-NB	-2.90	107.83	110.52
25	S	615	LUT	C40-C33-C34	-2.90	118.86	122.92
24	c	502	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	AB	309	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	v	615	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	1	508	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	BQ	609	CHL	CHC-C4B-NB	-2.90	121.19	124.26
38	A	408	PHO	O2D-CGD-O1D	-2.90	118.17	123.84
25	8	311	LUT	C40-C33-C34	-2.90	118.86	122.92
25	r	615	LUT	C40-C33-C34	-2.90	118.86	122.92
24	BU	608	CLA	C3B-C4B-NB	-2.90	107.83	110.52
23	7	310	CHL	CMD-C2D-C3D	-2.90	120.95	127.61
24	BB	313	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	B	608	CLA	C3B-C4B-NB	-2.89	107.83	110.52
25	G	615	LUT	C32-C33-C34	2.89	123.38	118.94
24	r	602	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	BE	605	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	Y	302	CHL	O2A-CGA-CBA	2.89	120.99	111.91
29	Bb	101	BCR	C33-C5-C6	-2.89	121.28	124.53
23	6	601	CHL	C3B-C4B-NB	2.89	113.20	110.52
24	B	610	CLA	C3B-C4B-NB	-2.89	107.83	110.52
24	BE	613	CLA	C3B-C4B-NB	-2.89	107.83	110.52
24	1	509	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
26	AA	319	NEX	C32-C33-C34	2.89	123.38	118.94
26	7	319	NEX	C32-C33-C34	2.89	123.38	118.94
32	a	412	SQD	O9-S-C6	2.89	110.38	106.94
23	BB	309	CHL	CMB-C2B-C1B	2.89	129.77	125.37
24	v	607	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	S	607	CHL	CMB-C2B-C1B	2.89	129.77	125.37
24	AB	301	CLA	CHB-C4A-NA	2.89	128.51	124.51
23	s	605	CHL	CMB-C2B-C1B	2.89	129.77	125.37
23	A2	608	CHL	C4-C3-C5	2.89	120.13	115.27
24	AA	315	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	Au	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	N	606	CHL	O2A-CGA-CBA	2.89	120.97	111.91
24	v	608	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	Bb	101	BCR	C27-C26-C25	2.89	126.92	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	610	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	BU	602	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	b	605	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	BQ	608	CHL	C4-C3-C5	2.89	120.13	115.27
24	a	410	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
25	Y	316	LUT	C35-C15-C14	2.89	129.38	123.47
23	Au	607	CHL	C4-C3-C5	2.88	120.12	115.27
23	y	308	CHL	C4-C3-C5	2.88	120.12	115.27
23	BQ	606	CHL	C3B-C4B-NB	2.88	113.19	110.52
25	BJ	616	LUT	C40-C33-C34	-2.88	118.89	122.92
23	7	306	CHL	C3B-C4B-NB	2.88	113.19	110.52
24	BF	514	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	v	603	CLA	C3B-C4B-NB	-2.88	107.84	110.52
38	A	409	PHO	O2D-CGD-O1D	-2.88	118.20	123.84
23	A2	606	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
23	A6	607	CHL	OMC-CMC-C2C	-2.88	119.17	125.69
24	5	610	CLA	CMC-C2C-C1C	2.88	129.42	125.04
23	6	605	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
24	BF	514	CLA	CHB-C4A-NA	2.88	128.49	124.51
23	Y	306	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
24	B	615	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	C	508	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	G	615	LUT	C35-C15-C14	2.88	129.37	123.47
31	D	403	PL9	C40-C39-C41	2.88	120.11	115.27
23	Ba	309	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
24	8	309	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	N	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	Ba	311	CLA	C3B-C4B-NB	-2.88	107.85	110.52
23	8	304	CHL	CMD-C2D-C3D	-2.88	121.00	127.61
23	s	605	CHL	C2D-C1D-ND	2.88	112.22	110.10
23	y	309	CHL	C3D-C4D-ND	2.88	114.89	110.24
24	1	512	CLA	C3B-C4B-NB	-2.88	107.85	110.52
23	A2	606	CHL	O2A-CGA-CBA	2.88	120.93	111.91
23	0	608	CHL	CMD-C2D-C3D	-2.88	121.00	127.61
24	N	613	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	z	102	BCR	C27-C26-C25	2.87	126.91	122.73
24	v	610	CLA	C3B-C4B-NB	-2.87	107.85	110.52
24	BQ	603	CLA	C3B-C4B-NB	-2.87	107.85	110.52
25	Au	615	LUT	C32-C33-C34	2.87	123.35	118.94
31	2	404	PL9	C40-C39-C41	2.87	120.11	115.27
25	Y	317	LUT	C40-C33-C34	-2.87	118.90	122.92
24	BJ	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Au	619	XAT	C40-C33-C32	-2.87	113.55	118.08
23	Ba	306	CHL	CMB-C2B-C1B	2.87	129.75	125.37
24	9	604	CLA	C1-C2-C3	-2.87	122.10	126.75
23	7	307	CHL	C3D-C4D-ND	2.87	114.89	110.24
23	g	609	CHL	C3D-C4D-ND	2.87	114.88	110.24
28	AA	301	XAT	C12-C13-C14	-2.87	114.53	118.94
28	BQ	619	XAT	C40-C33-C32	-2.87	113.55	118.08
23	BB	310	CHL	O2D-CGD-O1D	-2.87	118.22	123.84
24	7	315	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	AB	304	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
34	BF	517	DGD	CDB-CCB-CBB	-2.87	99.85	114.42
24	v	613	CLA	C3B-C4B-NB	-2.87	107.85	110.52
23	BJ	607	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
23	BJ	607	CHL	CHB-C1B-NB	-2.87	121.22	124.26
24	1	506	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	BD	410	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	AA	307	CHL	C3D-C4D-ND	2.87	114.88	110.24
24	BB	314	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
28	9	619	XAT	C38-C25-C24	-2.87	111.05	114.28
29	v	619	BCR	C24-C23-C22	-2.87	121.90	126.23
26	A2	617	NEX	C16-C1-C6	2.87	113.04	110.47
24	G	612	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	H	101	BCR	C24-C23-C22	-2.87	121.90	126.23
23	6	606	CHL	C3D-C4D-ND	2.87	114.87	110.24
23	r	605	CHL	C3D-C4D-ND	2.87	114.87	110.24
24	Y	313	CLA	CHB-C4A-NA	2.87	128.47	124.51
24	g	604	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	N	609	CHL	C1-C2-C3	-2.87	121.09	126.04
23	N	606	CHL	CMD-C2D-C3D	-2.87	121.02	127.61
29	b	618	BCR	C33-C5-C6	-2.86	121.31	124.53
23	g	608	CHL	OMC-CMC-C2C	-2.86	119.21	125.69
23	r	605	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
24	7	312	CLA	C3B-C4B-NB	-2.86	107.86	110.52
34	c	516	DGD	CDB-CCB-CBB	-2.86	99.89	114.42
23	Au	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
24	1	505	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	G	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	Au	609	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	A2	607	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	g	607	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
23	AB	307	CHL	CHD-C4C-C3C	-2.86	120.63	124.84
24	a	405	CLA	C3B-C4B-NB	-2.86	107.86	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	g	605	CHL	CMB-C2B-C1B	2.86	129.73	125.37
23	s	607	CHL	C3D-C4D-ND	2.86	114.86	110.24
23	N	607	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	N	608	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	G	609	CHL	C1-C2-C3	-2.86	121.10	126.04
30	A0	201	LMG	O6-C1-O1	-2.86	103.20	109.97
24	BV	609	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	Au	603	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	AA	310	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
25	BU	615	LUT	C12-C13-C14	2.86	123.33	118.94
24	B	612	CLA	C3B-C4B-NB	-2.86	107.86	110.52
23	0	606	CHL	C3D-C4D-ND	2.86	114.86	110.24
24	G	610	CLA	C1-C2-C3	-2.86	121.10	126.04
23	Au	607	CHL	O2A-CGA-CBA	2.86	120.88	111.91
23	BV	605	CHL	C1D-ND-C4D	-2.86	104.31	106.33
24	A6	602	CLA	CHB-C4A-NA	2.86	128.46	124.51
24	2	403	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	s	606	CHL	CMB-C2B-C1B	2.86	129.72	125.37
24	BJ	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	BJ	615	LUT	C15-C35-C34	2.86	129.32	123.47
24	c	514	CLA	CHB-C4A-NA	2.86	128.46	124.51
23	Y	308	CHL	O2A-CGA-CBA	2.86	120.87	111.91
24	s	610	CLA	C3B-C4B-NB	-2.86	107.87	110.52
30	BL	101	LMG	O6-C1-O1	-2.86	103.21	109.97
24	B	607	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
24	AB	308	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
23	BQ	606	CHL	CMD-C2D-C3D	-2.85	121.05	127.61
23	BV	607	CHL	C3D-C4D-ND	2.85	114.85	110.24
23	n	601	CHL	O2A-CGA-CBA	2.85	120.86	111.91
24	BE	614	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	1	515	BCR	C15-C16-C17	-2.85	117.63	123.47
23	g	609	CHL	C6-C5-C3	-2.85	109.95	114.62
23	BB	308	CHL	O2A-CGA-CBA	2.85	120.86	111.91
24	a	406	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	BD	412	SQD	O9-S-C6	2.85	110.33	106.94
29	C	515	BCR	C15-C16-C17	-2.85	117.63	123.47
24	BF	504	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	B	617	BCR	C33-C5-C6	-2.85	121.33	124.53
23	s	605	CHL	C1D-ND-C4D	-2.85	104.31	106.33
24	c	503	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	y	306	CHL	CMB-C2B-C1B	2.85	129.71	125.37
24	BF	505	CLA	O2D-CGD-O1D	-2.85	118.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	520	LHG	O8-C23-C24	2.85	120.85	111.91
23	BQ	607	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
23	y	302	CHL	C1D-ND-C4D	-2.85	104.31	106.33
24	b	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	v	612	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	K	102	BCR	C24-C23-C22	-2.85	121.93	126.23
23	Ba	308	CHL	C1-C2-C3	-2.85	121.12	126.04
23	A2	608	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
25	A6	615	LUT	C1-C6-C5	-2.85	118.60	122.61
24	s	613	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	AA	313	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	BD	407	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	0	602	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
34	1	516	DGD	CDB-CCB-CBB	-2.85	99.97	114.42
24	b	610	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	n	606	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
25	7	316	LUT	C40-C33-C34	-2.85	118.93	122.92
23	AB	305	CHL	CMB-C2B-C1B	2.85	129.71	125.37
31	2	404	PL9	C7-C8-C9	-2.85	122.05	126.79
23	N	609	CHL	CMB-C2B-C1B	2.85	129.71	125.37
23	r	607	CHL	CMB-C2B-C1B	2.85	129.71	125.37
23	n	608	CHL	C3D-C4D-ND	2.85	114.84	110.24
24	S	608	CLA	C3B-C4B-NB	-2.85	107.88	110.52
24	1	507	CLA	C3B-C4B-NB	-2.85	107.88	110.52
23	BV	607	CHL	CMB-C2B-C1B	2.85	129.70	125.37
23	y	310	CHL	C6-C5-C3	-2.85	109.97	114.62
24	BF	513	CLA	C1-C2-C3	-2.85	121.12	126.04
23	Au	606	CHL	C3D-C4D-ND	2.85	114.84	110.24
23	BJ	605	CHL	CMB-C2B-C1B	2.85	129.70	125.37
23	g	608	CHL	CHB-C4A-NA	2.84	128.45	124.51
28	AB	312	XAT	C5-C4-C3	-2.84	107.12	112.75
23	y	308	CHL	C1-C2-C3	-2.84	121.12	126.04
25	BB	316	LUT	C35-C15-C14	2.84	129.30	123.47
24	n	603	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	g	608	CHL	CMB-C2B-C1B	2.84	129.70	125.37
24	D	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	G	601	CHL	CHB-C4A-NA	2.84	128.44	124.51
23	9	605	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
38	R	408	PHO	O2D-CGD-O1D	-2.84	118.28	123.84
23	Au	601	CHL	O2A-CGA-CBA	2.84	120.83	111.91
23	s	601	CHL	C1D-ND-C4D	-2.84	104.32	106.33
23	Ba	306	CHL	CMD-C2D-C3D	-2.84	121.08	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BU	605	CHL	C3D-C4D-ND	2.84	114.83	110.24
23	BQ	601	CHL	O2A-CGA-CBA	2.84	120.83	111.91
24	BV	610	CLA	C3B-C4B-NB	-2.84	107.88	110.52
29	4	101	BCR	C33-C5-C6	-2.84	121.34	124.53
24	Ba	312	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	F	101	BCR	C33-C5-C6	-2.84	121.34	124.53
24	8	301	CLA	CHB-C4A-NA	2.84	128.44	124.51
32	a	412	SQD	O8-S-C6	2.84	110.27	105.74
29	z	102	BCR	C15-C16-C17	-2.84	117.66	123.47
24	7	303	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	A6	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	Au	610	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	Ba	310	CHL	CAC-C3C-C4C	2.84	128.49	124.81
25	6	615	LUT	C40-C33-C34	-2.84	118.95	122.92
24	7	305	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	S	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	BU	607	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
24	1	513	CLA	C3B-C4B-NB	-2.84	107.88	110.52
34	a	401	DGD	CDB-CCB-CBB	-2.84	100.03	114.42
23	Ba	302	CHL	O2A-CGA-CBA	2.84	120.81	111.91
25	G	616	LUT	C15-C35-C34	2.84	129.28	123.47
24	Au	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	9	616	LUT	C39-C29-C28	2.84	122.54	118.08
24	1	509	CLA	C3B-C4B-NB	-2.83	107.89	110.52
34	C	516	DGD	CDB-CCB-CBB	-2.83	100.03	114.42
24	v	609	CLA	CHB-C4A-NA	2.83	128.43	124.51
34	BD	401	DGD	CDB-CCB-CBB	-2.83	100.03	114.42
23	BJ	608	CHL	OMC-CMC-C2C	-2.83	119.28	125.69
23	A2	608	CHL	C3D-C4D-ND	2.83	114.82	110.24
24	y	312	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	BE	622	LHG	O8-C23-C24	2.83	120.80	111.91
23	S	607	CHL	C3B-C4B-NB	2.83	113.14	110.52
24	b	617	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	BV	606	CHL	CMB-C2B-C1B	2.83	129.69	125.37
23	0	601	CHL	C4-C3-C5	2.83	120.04	115.27
23	Y	310	CHL	C4-C3-C5	2.83	120.04	115.27
24	G	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	n	602	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	5	619	XAT	C38-C25-C24	-2.83	111.09	114.28
23	y	302	CHL	O2A-CGA-CBA	2.83	120.80	111.91
23	A2	609	CHL	C4-C3-C5	2.83	120.03	115.27
23	BU	607	CHL	CMB-C2B-C1B	2.83	129.68	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	604	CLA	C1-C2-C3	-2.83	122.17	126.75
24	BD	406	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	G	606	CHL	C3D-C4D-ND	2.83	114.82	110.24
25	BU	615	LUT	C15-C35-C34	2.83	129.27	123.47
24	c	510	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	BB	310	CHL	C4-C3-C5	2.83	120.03	115.27
24	A2	603	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	7	309	CHL	CMB-C2B-C1B	2.83	129.68	125.37
25	A6	614	LUT	C35-C15-C14	2.83	129.27	123.47
24	B	613	CLA	CHB-C4A-NA	2.83	128.43	124.51
33	F	102	HEM	C4A-NA-C1A	2.83	108.12	105.35
24	b	614	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	c	504	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	BF	508	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
33	4	102	HEM	C4A-NA-C1A	2.83	108.12	105.35
23	8	305	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	s	608	CLA	C3B-C4B-NB	-2.83	107.89	110.52
24	BU	603	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	6	608	CHL	C3D-C4D-ND	2.83	114.81	110.24
23	BJ	608	CHL	CHB-C4A-NA	2.83	128.42	124.51
24	N	603	CLA	C3B-C4B-NB	-2.83	107.89	110.52
24	C	507	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	BJ	609	CHL	C6-C5-C3	-2.83	110.00	114.62
24	7	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	BJ	607	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
28	BQ	619	XAT	C20-C13-C12	-2.83	113.62	118.08
24	1	513	CLA	CHB-C4A-NA	2.83	128.42	124.51
34	h	102	DGD	CDB-CCB-CBB	-2.82	100.08	114.42
24	R	409	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
24	r	603	CLA	C3B-C4B-NB	-2.82	107.89	110.52
24	AA	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
24	AA	304	CLA	C3B-C4B-NB	-2.82	107.90	110.52
23	Y	302	CHL	C4-C3-C5	2.82	120.02	115.27
24	A2	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	A2	609	CHL	CMB-C2B-C1B	2.82	129.67	125.37
23	y	307	CHL	C4A-NA-C1A	2.82	107.97	106.71
23	N	605	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
24	AB	310	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	G	607	CHL	O2A-CGA-CBA	2.82	120.76	111.91
24	B	613	CLA	C3B-C4B-NB	-2.82	107.90	110.52
23	G	607	CHL	C4-C3-C5	2.82	120.02	115.27
24	g	603	CLA	O2D-CGD-O1D	-2.82	118.32	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A6	607	CHL	CHC-C4B-NB	-2.82	121.27	124.26
24	7	304	CLA	C3B-C4B-NB	-2.82	107.90	110.52
24	g	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	BQ	608	CHL	C3D-C4D-ND	2.82	114.80	110.24
24	6	602	CLA	CHB-C4A-NA	2.82	128.41	124.51
32	L	101	SQD	O7-S-C6	2.82	110.29	106.94
24	g	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	Ba	303	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	5	605	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
23	G	609	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
24	9	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	BQ	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	g	609	CHL	C4-C3-C5	2.82	120.01	115.27
38	A	408	PHO	O1D-CGD-CBD	2.82	129.43	124.74
31	BG	403	PL9	C22-C23-C24	-2.81	120.88	127.66
24	N	604	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	AA	303	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
27	BF	521	LHG	O8-C23-C24	2.81	120.74	111.91
24	C	505	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	BQ	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	6	615	LUT	C20-C13-C14	-2.81	118.98	122.92
23	y	310	CHL	O2D-CGD-O1D	-2.81	118.34	123.84
24	C	511	CLA	C1D-ND-C4D	2.81	108.33	106.33
24	B	615	CLA	CHB-C4A-NA	2.81	128.40	124.51
24	C	513	CLA	CHB-C4A-NA	2.81	128.40	124.51
30	i	101	LMG	O6-C1-O1	-2.81	103.31	109.97
23	g	601	CHL	CMB-C2B-C1B	2.81	129.65	125.37
23	6	607	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
23	A2	609	CHL	C1-C2-C3	-2.81	121.18	126.04
23	BJ	601	CHL	CMB-C2B-C1B	2.81	129.65	125.37
23	BQ	606	CHL	C4A-NA-C1A	2.81	107.97	106.71
23	Au	608	CHL	C1D-ND-C4D	-2.81	104.34	106.33
34	1	517	DGD	CDB-CCB-CBB	-2.81	100.15	114.42
24	B	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	A	410	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	1	504	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	8	312	XAT	C40-C33-C32	-2.81	113.65	118.08
23	G	607	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
29	1	514	BCR	C33-C5-C6	-2.81	121.37	124.53
23	N	608	CHL	C3D-C4D-ND	2.81	114.78	110.24
23	s	607	CHL	CMB-C2B-C1B	2.81	129.65	125.37
32	L	101	SQD	O5-C5-C4	2.81	114.80	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	614	LUT	C40-C33-C34	-2.81	118.99	122.92
23	BQ	601	CHL	CMB-C2B-C1B	2.81	129.65	125.37
24	r	610	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	n	607	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
24	BE	610	CLA	CHB-C4A-NA	2.81	128.40	124.51
24	N	614	CLA	C3B-C4B-NB	-2.81	107.91	110.52
24	BE	617	CLA	C3B-C4B-NB	-2.81	107.91	110.52
24	B	608	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	0	614	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	BJ	612	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	A2	606	CHL	C3D-C4D-ND	2.81	114.78	110.24
23	y	310	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
23	r	606	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
24	Y	311	CLA	CMC-C2C-C1C	2.81	129.31	125.04
25	7	317	LUT	C40-C33-C34	-2.81	118.99	122.92
24	6	614	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	c	514	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	r	608	CLA	C3B-C4B-NB	-2.81	107.91	110.52
27	BE	623	LHG	O8-C23-C24	2.81	120.72	111.91
23	n	601	CHL	CMB-C2B-C1B	2.81	129.64	125.37
24	BE	602	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
34	H	102	DGD	CDB-CCB-CBB	-2.81	100.18	114.42
24	1	502	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	9	601	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
24	s	610	CLA	CHB-C4A-NA	2.81	128.39	124.51
24	A6	603	CLA	CHB-C4A-NA	2.81	128.39	124.51
27	BQ	618	LHG	O8-C23-C24	2.80	120.71	111.91
23	y	309	CHL	C3B-C4B-NB	2.80	113.12	110.52
24	A6	608	CLA	C3B-C4B-NB	-2.80	107.91	110.52
23	5	608	CHL	OMC-CMC-C2C	-2.80	119.35	125.69
24	BJ	613	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	y	302	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
24	b	611	CLA	CHB-C4A-NA	2.80	128.39	124.51
24	a	407	CLA	CHB-C4A-NA	2.80	128.39	124.51
24	Y	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	BQ	605	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
23	BQ	605	CHL	CMB-C2B-C1B	2.80	129.64	125.37
23	6	609	CHL	CHD-C4C-C3C	-2.80	120.72	124.84
23	y	310	CHL	CHD-C4C-C3C	-2.80	120.72	124.84
24	AA	312	CLA	CHB-C4A-NA	2.80	128.39	124.51
24	BV	610	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	A	412	LMG	O6-C1-O1	-2.80	103.34	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Au	607	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
25	7	317	LUT	C35-C15-C14	2.80	129.21	123.47
23	G	601	CHL	O2A-CGA-CBA	2.80	120.70	111.91
27	b	622	LHG	O8-C23-C24	2.80	120.70	111.91
23	BJ	608	CHL	CMB-C2B-C1B	2.80	129.64	125.37
38	R	407	PHO	O1D-CGD-CBD	2.80	129.41	124.74
24	C	513	CLA	C3B-C4B-NB	-2.80	107.92	110.52
24	B	611	CLA	CHB-C4A-NA	2.80	128.39	124.51
24	s	602	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	g	607	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
24	r	611	CLA	C3B-C4B-NB	-2.80	107.92	110.52
23	BB	308	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
23	Ba	302	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
28	A2	619	XAT	C12-C13-C14	-2.80	114.64	118.94
24	Au	610	CLA	CHB-C4A-NA	2.80	128.38	124.51
24	C	506	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	BE	618	BCR	C15-C16-C17	-2.80	117.74	123.47
24	b	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
24	b	604	CLA	C3B-C4B-NB	-2.80	107.92	110.52
24	6	602	CLA	CHB-C1B-NB	2.80	127.22	124.26
23	9	608	CHL	OMC-CMC-C2C	-2.80	119.36	125.69
24	AA	312	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
26	BQ	617	NEX	C28-C29-C30	2.80	123.23	118.94
24	I	102	CLA	C3B-C4B-NB	-2.80	107.92	110.52
23	6	607	CHL	C1D-ND-C4D	-2.80	104.35	106.33
25	g	615	LUT	C15-C35-C34	2.80	129.20	123.47
24	B	605	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
24	C	511	CLA	C2D-C1D-ND	-2.80	108.04	110.10
24	S	602	CLA	C3B-C4B-NB	-2.80	107.92	110.52
24	0	610	CLA	O2A-CGA-O1A	-2.80	116.54	123.59
25	Au	615	LUT	C35-C15-C14	2.80	129.20	123.47
25	BU	615	LUT	C35-C15-C14	2.80	129.20	123.47
24	v	605	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	A2	605	CHL	CMD-C2D-C3D	-2.80	121.18	127.61
34	a	413	DGD	O5D-C6D-C5D	-2.80	103.87	109.05
25	S	615	LUT	C39-C29-C28	2.80	122.48	118.08
32	L	103	SQD	O8-S-C6	2.79	110.19	105.74
25	S	615	LUT	C1-C6-C5	-2.79	118.68	122.61
24	g	612	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
24	a	405	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
23	S	601	CHL	CMB-C2B-C1B	2.79	129.62	125.37
23	7	306	CHL	C3D-C4D-ND	2.79	114.76	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	607	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
24	v	611	CLA	CHB-C4A-NA	2.79	128.38	124.51
25	A6	615	LUT	C20-C13-C14	-2.79	119.01	122.92
24	G	611	CLA	C3B-C4B-NB	-2.79	107.92	110.52
23	5	609	CHL	C4-C3-C5	2.79	119.97	115.27
23	y	306	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
23	5	609	CHL	CMB-C2B-C1B	2.79	129.62	125.37
29	b	618	BCR	C15-C16-C17	-2.79	117.75	123.47
23	Au	606	CHL	CHB-C4A-NA	2.79	128.38	124.51
23	AA	309	CHL	CMB-C2B-C1B	2.79	129.62	125.37
24	n	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	5	601	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
29	K	102	BCR	C33-C5-C6	-2.79	121.39	124.53
24	C	504	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	Y	309	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
24	1	510	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	AA	308	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
23	Y	310	CHL	C1-C2-C3	-2.79	121.22	126.04
23	8	307	CHL	CMB-C2B-C1B	2.79	129.62	125.37
23	0	605	CHL	CMB-C2B-C1B	2.79	129.62	125.37
24	N	610	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	c	509	CLA	C3B-C4B-NB	-2.79	107.93	110.52
25	BV	614	LUT	C40-C33-C34	-2.79	119.01	122.92
23	g	608	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
23	n	605	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
23	BJ	609	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
27	1	521	LHG	O8-C23-C24	2.79	120.66	111.91
25	Y	317	LUT	C12-C13-C14	2.79	123.22	118.94
24	5	614	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	S	602	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	A6	601	CHL	CMB-C2B-C1B	2.79	129.62	125.37
38	R	408	PHO	CMB-C2B-C3B	2.79	129.89	124.68
23	7	310	CHL	C3D-C4D-ND	2.79	114.75	110.24
23	0	608	CHL	C3D-C4D-ND	2.79	114.75	110.24
24	Y	304	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	Aw	102	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	BF	510	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	y	310	CHL	CMB-C2B-C1B	2.79	129.61	125.37
23	G	606	CHL	CMB-C2B-C1B	2.79	129.61	125.37
23	Ba	310	CHL	CMB-C2B-C1B	2.79	129.61	125.37
30	Aw	101	LMG	O6-C1-O1	-2.79	103.38	109.97
24	9	614	CLA	CHB-C4A-NA	2.79	128.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A6	609	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	Av	101	BCR	C24-C23-C22	-2.79	122.03	126.23
23	AA	308	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
23	BB	302	CHL	C4-C3-C5	2.79	119.96	115.27
24	S	609	CLA	CHB-C4A-NA	2.79	128.36	124.51
24	BE	611	CLA	CHB-C4A-NA	2.79	128.36	124.51
25	BQ	616	LUT	C40-C33-C34	-2.79	119.02	122.92
24	BF	511	CLA	C3B-C4B-NB	-2.79	107.93	110.52
23	6	605	CHL	CMB-C2B-C1B	2.79	129.61	125.37
24	BF	513	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	G	606	CHL	CHB-C4A-NA	2.78	128.36	124.51
23	G	605	CHL	C1C-C2C-C3C	-2.78	104.90	107.11
23	Au	609	CHL	C1C-C2C-C3C	-2.78	104.90	107.11
24	y	303	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
24	BD	405	CLA	C3B-C4B-NB	-2.78	107.93	110.52
23	BJ	606	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
24	G	604	CLA	C1-C2-C3	-2.78	122.25	126.75
24	v	606	CLA	CHB-C4A-NA	2.78	128.36	124.51
24	r	614	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	s	606	CHL	O1D-CGD-CBD	-2.78	118.79	124.48
24	Au	611	CLA	C3B-C4B-NB	-2.78	107.93	110.52
24	BD	407	CLA	C1-C2-C3	-2.78	122.25	126.75
23	N	609	CHL	C4-C3-C5	2.78	119.95	115.27
23	Y	306	CHL	O2A-CGA-CBA	2.78	120.64	111.91
23	7	308	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
34	C	517	DGD	CDB-CCB-CBB	-2.78	100.30	114.42
24	S	604	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	5	606	CHL	C2A-C1A-CHA	-2.78	118.99	123.86
23	9	606	CHL	C2A-C1A-CHA	-2.78	118.99	123.86
24	BE	604	CLA	C3B-C4B-NB	-2.78	107.93	110.52
28	AA	301	XAT	C40-C33-C32	-2.78	113.69	118.08
24	BJ	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	N	619	XAT	C12-C13-C14	-2.78	114.67	118.94
24	y	303	CLA	C3B-C4B-NB	-2.78	107.94	110.52
24	2	403	CLA	C3B-C4B-NB	-2.78	107.94	110.52
23	7	308	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
23	BV	605	CHL	C2D-C1D-ND	2.78	112.15	110.10
27	C	521	LHG	O8-C23-C24	2.78	120.63	111.91
24	A6	604	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	BU	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	N	601	CHL	C1-C2-C3	-2.78	121.23	126.04
23	AA	307	CHL	CMD-C2D-C3D	-2.78	121.22	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	609	CHL	C4-C3-C5	2.78	119.95	115.27
23	BU	606	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
23	BJ	608	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
24	AA	303	CLA	C3B-C4B-NB	-2.78	107.94	110.52
23	n	608	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
23	g	601	CHL	C4-C3-C5	2.78	119.94	115.27
23	n	605	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
23	Ba	310	CHL	O2D-CGD-O1D	-2.78	118.41	123.84
23	A2	601	CHL	O2A-CGA-CBA	2.78	120.62	111.91
24	BF	509	CLA	CHB-C4A-NA	2.78	128.35	124.51
24	s	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
24	BU	611	CLA	C3B-C4B-NB	-2.78	107.94	110.52
23	BV	606	CHL	C4-C3-C5	2.78	119.94	115.27
23	8	306	CHL	CAA-CBA-CGA	-2.78	105.14	112.51
34	BD	413	DGD	O5D-C6D-C5D	-2.78	103.91	109.05
23	9	607	CHL	C1D-ND-C4D	-2.78	104.36	106.33
23	n	606	CHL	C3D-C4D-ND	2.78	114.73	110.24
24	b	616	CLA	C3B-C4B-NB	-2.78	107.94	110.52
24	C	509	CLA	C3B-C4B-NB	-2.78	107.94	110.52
24	C	512	CLA	C3B-C4B-NB	-2.78	107.94	110.52
24	Ba	304	CLA	C3B-C4B-NB	-2.78	107.94	110.52
23	N	601	CHL	O2A-CGA-CBA	2.78	120.62	111.91
27	BJ	618	LHG	O8-C23-C24	2.78	120.62	111.91
34	Av	102	DGD	CDB-CCB-CBB	-2.78	100.34	114.42
29	Ay	102	BCR	C24-C23-C22	-2.77	122.04	126.23
25	BJ	615	LUT	C12-C13-C14	2.77	123.20	118.94
27	n	618	LHG	O8-C23-C24	2.77	120.61	111.91
24	5	611	CLA	C3B-C4B-NB	-2.77	107.94	110.52
24	Ba	303	CLA	C3B-C4B-NB	-2.77	107.94	110.52
23	BV	606	CHL	O1D-CGD-CBD	-2.77	118.81	124.48
24	1	511	CLA	O2D-CGD-CBD	2.77	116.20	111.27
24	Au	602	CLA	C3B-C4B-NB	-2.77	107.94	110.52
24	BE	616	CLA	C3B-C4B-NB	-2.77	107.94	110.52
23	Ba	309	CHL	C3B-C4B-NB	2.77	113.09	110.52
23	9	609	CHL	C4-C3-C5	2.77	119.94	115.27
32	A1	101	SQD	O8-S-C6	2.77	110.16	105.74
38	A	409	PHO	CMB-C2B-C3B	2.77	129.87	124.68
24	5	613	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	Ba	302	CHL	CMB-C2B-C1B	2.77	129.59	125.37
23	Ba	307	CHL	C4A-NA-C1A	2.77	107.95	106.71
24	c	512	CLA	C3B-C4B-NB	-2.77	107.94	110.52
24	0	611	CLA	C3B-C4B-NB	-2.77	107.94	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	614	CLA	CHB-C4A-NA	2.77	128.34	124.51
34	c	516	DGD	C3G-C2G-C1G	-2.77	105.23	111.79
25	A2	615	LUT	C12-C13-C14	2.77	123.19	118.94
24	c	502	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	BB	302	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
28	AB	312	XAT	C40-C33-C32	-2.77	113.71	118.08
29	BI	101	BCR	C33-C5-C6	-2.77	121.42	124.53
23	9	607	CHL	CMB-C2B-C1B	2.77	129.59	125.37
23	BJ	608	CHL	O2A-CGA-CBA	2.77	120.60	111.91
24	A2	611	CLA	C3B-C4B-NB	-2.77	107.95	110.52
24	BV	608	CLA	C3B-C4B-NB	-2.77	107.95	110.52
24	N	604	CLA	C1-C2-C3	-2.77	122.27	126.75
23	AA	310	CHL	C3D-C4D-ND	2.77	114.72	110.24
23	g	606	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
24	Au	612	CLA	C3B-C4B-NB	-2.77	107.95	110.52
23	s	606	CHL	C4-C3-C5	2.77	119.92	115.27
28	7	301	XAT	C40-C33-C32	-2.77	113.72	118.08
23	A6	606	CHL	CHB-C4A-NA	2.77	128.34	124.51
24	7	312	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	b	613	CLA	C3B-C4B-NB	-2.77	107.95	110.52
23	g	609	CHL	C1C-C2C-C3C	-2.77	104.92	107.11
25	A2	616	LUT	C12-C13-C14	2.77	123.19	118.94
23	Y	308	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
27	g	618	LHG	O8-C23-C24	2.77	120.58	111.91
24	d	401	CLA	C3B-C4B-NB	-2.76	107.95	110.52
31	2	404	PL9	C22-C23-C24	-2.76	121.00	127.66
24	BV	608	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
24	BF	505	CLA	C3B-C4B-NB	-2.76	107.95	110.52
23	y	310	CHL	C4-C3-C5	2.76	119.92	115.27
27	G	618	LHG	O8-C23-C24	2.76	120.58	111.91
23	AA	308	CHL	CHB-C4A-NA	2.76	128.33	124.51
29	B	617	BCR	C24-C23-C22	-2.76	122.06	126.23
23	g	601	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
24	S	603	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	N	606	CHL	C3D-C4D-ND	2.76	114.70	110.24
30	BE	621	LMG	O6-C1-O1	-2.76	103.44	109.97
23	BQ	608	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
24	BD	407	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	7	310	CHL	C3B-C4B-NB	2.76	113.08	110.52
24	s	603	CLA	C3B-C4B-NB	-2.76	107.95	110.52
24	A6	610	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	Ba	310	CHL	CHD-C4C-C3C	-2.76	120.78	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	603	CLA	C3B-C4B-NB	-2.76	107.96	110.52
23	BJ	601	CHL	C1C-C2C-C3C	-2.76	104.92	107.11
23	7	307	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
23	e	601	CHL	CMB-C2B-C1B	2.76	129.57	125.37
28	Y	301	XAT	C12-C13-C14	-2.76	114.71	118.94
23	g	608	CHL	O2A-CGA-CBA	2.76	120.56	111.91
29	z	102	BCR	C33-C5-C6	-2.76	121.43	124.53
23	A2	609	CHL	C1C-C2C-C3C	-2.76	104.93	107.11
29	Ay	102	BCR	C27-C26-C25	2.76	126.73	122.73
24	R	406	CLA	C1-C2-C3	-2.76	122.29	126.75
23	BB	306	CHL	O2A-CGA-CBA	2.76	120.56	111.91
23	BJ	605	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
38	BD	409	PHO	O1D-CGD-CBD	2.76	129.33	124.74
24	B	609	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	1	510	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	BE	611	CLA	C3B-C4B-NB	-2.75	107.96	110.52
25	r	615	LUT	C12-C13-C14	2.75	123.17	118.94
23	AB	307	CHL	CMB-C2B-C1B	2.75	129.56	125.37
25	BU	615	LUT	C7-C8-C9	-2.75	122.07	126.23
25	y	317	LUT	C15-C35-C34	2.75	129.11	123.47
23	n	605	CHL	CMB-C2B-C1B	2.75	129.56	125.37
23	BQ	605	CHL	CHB-C4A-NA	2.75	128.32	124.51
24	6	610	CLA	C2A-C3A-C4A	2.75	106.32	101.87
24	BQ	614	CLA	C3B-C4B-NB	-2.75	107.96	110.52
29	h	101	BCR	C15-C14-C13	-2.75	123.38	127.31
29	H	101	BCR	C27-C26-C25	2.75	126.73	122.73
29	8	313	BCR	C33-C5-C6	-2.75	121.44	124.53
24	A2	614	CLA	C3B-C4B-NB	-2.75	107.96	110.52
23	n	609	CHL	C4-C3-C5	2.75	119.90	115.27
29	b	620	BCR	C33-C5-C6	-2.75	121.44	124.53
31	D	403	PL9	C7-C3-C2	-2.75	119.68	123.30
24	v	615	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	AB	313	BCR	C11-C10-C9	-2.75	123.38	127.31
25	Au	615	LUT	C8-C9-C10	2.75	123.16	118.94
23	BJ	601	CHL	C4-C3-C5	2.75	119.90	115.27
23	g	606	CHL	C3D-C4D-ND	2.75	114.69	110.24
23	Ba	309	CHL	C3D-C4D-ND	2.75	114.69	110.24
23	S	606	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
23	AB	307	CHL	C4A-NA-C1A	2.75	107.94	106.71
24	g	604	CLA	C1-C2-C3	-2.75	122.31	126.75
23	AA	306	CHL	C3D-C4D-ND	2.75	114.68	110.24
24	BE	609	CLA	CHB-C4A-NA	2.75	128.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	613	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
27	Au	618	LHG	O8-C23-C24	2.75	120.53	111.91
24	C	502	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
27	b	623	LHG	O8-C23-C24	2.75	120.53	111.91
24	b	614	CLA	C3B-C4B-NB	-2.75	107.97	110.52
23	e	601	CHL	CHB-C4A-NA	2.75	128.31	124.51
23	A2	606	CHL	C1D-ND-C4D	-2.75	104.38	106.33
23	A2	609	CHL	C1D-ND-C4D	-2.75	104.38	106.33
29	h	101	BCR	C27-C26-C25	2.75	126.72	122.73
24	BE	607	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
24	BF	510	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	BD	405	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
23	AB	306	CHL	CAA-CBA-CGA	-2.74	105.22	112.51
27	0	617	LHG	O8-C23-C24	2.74	120.52	111.91
24	D	402	CLA	C3B-C4B-NB	-2.74	107.97	110.52
23	g	609	CHL	CMB-C2B-C1B	2.74	129.55	125.37
29	BK	101	BCR	C15-C14-C13	-2.74	123.39	127.31
23	8	304	CHL	C3D-C4D-ND	2.74	114.67	110.24
23	n	605	CHL	CHB-C4A-NA	2.74	128.31	124.51
23	g	605	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
24	Ba	311	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	0	615	LUT	C8-C9-C10	2.74	123.15	118.94
23	BH	601	CHL	CMB-C2B-C1B	2.74	129.54	125.37
25	N	615	LUT	C32-C33-C34	2.74	123.15	118.94
24	BE	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	A6	606	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
23	BJ	601	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
25	7	316	LUT	C32-C33-C34	2.74	123.15	118.94
24	y	311	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	B	615	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	A2	610	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	Ba	315	CLA	C3B-C4B-NB	-2.74	107.97	110.52
23	BH	601	CHL	CHB-C4A-NA	2.74	128.30	124.51
24	B	606	CLA	CHB-C4A-NA	2.74	128.30	124.51
24	BE	606	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	C	507	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	N	615	LUT	C12-C13-C14	2.74	123.14	118.94
24	c	507	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
28	BB	301	XAT	C12-C13-C14	-2.74	114.74	118.94
24	1	508	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	BV	611	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
30	BG	405	LMG	O6-C1-O1	-2.74	103.49	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	s	601	CHL	CHC-C4B-NB	-2.74	121.36	124.26
23	A2	606	CHL	C3B-C4B-NB	2.74	113.05	110.52
24	5	611	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	BB	307	CHL	O2A-CGA-CBA	2.74	120.49	111.91
24	BE	617	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	G	612	CLA	C3B-C4B-NB	-2.74	107.98	110.52
24	n	611	CLA	CHB-C4A-NA	2.74	128.29	124.51
24	BF	514	CLA	C3B-C4B-NB	-2.73	107.98	110.52
25	A2	615	LUT	C32-C33-C34	2.73	123.14	118.94
24	0	612	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	y	308	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
25	6	616	LUT	C12-C13-C14	2.73	123.14	118.94
23	BB	310	CHL	C1-C2-C3	-2.73	121.31	126.04
24	s	608	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
30	BF	519	LMG	O6-C1-O1	-2.73	103.50	109.97
23	n	609	CHL	CMB-C2B-C1B	2.73	129.53	125.37
34	R	401	DGD	CDB-CCB-CBB	-2.73	100.55	114.42
23	BJ	606	CHL	C3D-C4D-ND	2.73	114.66	110.24
24	BJ	604	CLA	C1-C2-C3	-2.73	122.33	126.75
23	6	609	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
24	BB	313	CLA	C3B-C4B-NB	-2.73	107.98	110.52
23	BQ	609	CHL	CAC-C3C-C4C	2.73	128.35	124.81
24	0	602	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	g	615	LUT	C12-C13-C14	2.73	123.13	118.94
24	9	610	CLA	CHB-C1B-NB	2.73	127.15	124.26
25	9	615	LUT	C15-C35-C34	2.73	129.07	123.47
30	c	518	LMG	O6-C1-O1	-2.73	103.51	109.97
24	n	613	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	a	407	CLA	C1-C2-C3	-2.73	122.34	126.75
23	8	304	CHL	C4A-NA-C1A	2.73	107.93	106.71
24	c	509	CLA	CHB-C4A-NA	2.73	128.29	124.51
30	b	621	LMG	O6-C1-O1	-2.73	103.51	109.97
23	BV	601	CHL	CMB-C2B-C1B	2.73	129.53	125.37
24	BF	507	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	v	617	BCR	C24-C23-C22	-2.73	122.11	126.23
24	n	614	CLA	C3B-C4B-NB	-2.73	107.98	110.52
24	c	513	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	A2	605	CHL	O2A-CGA-CBA	2.73	120.47	111.91
24	Au	604	CLA	C1-C2-C3	-2.73	122.34	126.75
24	0	613	CLA	CAA-CBA-CGA	-2.73	105.28	113.25
24	b	606	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	BV	601	CHL	OMC-CMC-C2C	-2.73	119.52	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	613	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	g	605	CHL	CHB-C4A-NA	2.73	128.28	124.51
29	Av	101	BCR	C27-C26-C25	2.73	126.69	122.73
34	A	402	DGD	CDB-CCB-CBB	-2.73	100.58	114.42
23	9	609	CHL	CHD-C4C-C3C	-2.73	120.83	124.84
24	BQ	613	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
25	9	616	LUT	C32-C33-C34	2.73	123.12	118.94
24	G	610	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	Y	307	CHL	O2A-CGA-CBA	2.73	120.46	111.91
30	v	620	LMG	O6-C1-O1	-2.73	103.52	109.97
24	y	304	CLA	C3B-C4B-NB	-2.73	107.99	110.52
25	8	311	LUT	C12-C13-C14	2.73	123.12	118.94
23	Au	608	CHL	OMC-CMC-C2C	-2.73	119.52	125.69
24	6	602	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
25	S	615	LUT	C20-C13-C14	-2.73	119.11	122.92
24	BB	315	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	Ba	310	CHL	CMD-C2D-C3D	-2.73	121.34	127.61
29	f	101	BCR	C33-C5-C6	-2.72	121.47	124.53
29	v	618	BCR	C15-C16-C17	-2.72	117.89	123.47
24	G	603	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	A2	602	CLA	CHB-C4A-NA	2.72	128.28	124.51
24	BB	304	CLA	C3B-C4B-NB	-2.72	107.99	110.52
23	5	607	CHL	CMB-C2B-C1B	2.72	129.52	125.37
32	R	411	SQD	O8-S-C6	2.72	110.08	105.74
23	Y	302	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
23	y	302	CHL	CMB-C2B-C1B	2.72	129.52	125.37
24	S	604	CLA	C3B-C4B-NB	-2.72	107.99	110.52
24	c	506	CLA	C3B-C4B-NB	-2.72	107.99	110.52
25	A6	615	LUT	C39-C29-C28	2.72	122.37	118.08
24	BQ	610	CLA	C2A-C3A-C4A	2.72	106.27	101.87
24	G	611	CLA	O2D-CGD-CBD	2.72	116.11	111.27
23	Ba	308	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
29	BE	620	BCR	C33-C5-C6	-2.72	121.47	124.53
25	BB	317	LUT	C40-C33-C34	-2.72	119.11	122.92
23	BQ	609	CHL	C4-C3-C5	2.72	119.85	115.27
24	Y	305	CLA	C3B-C4B-NB	-2.72	107.99	110.52
24	Y	315	CLA	CHB-C4A-NA	2.72	128.28	124.51
24	b	607	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	AA	302	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
24	7	313	CLA	C3B-C4B-NB	-2.72	107.99	110.52
30	d	405	LMG	O6-C1-O1	-2.72	103.53	109.97
24	BQ	611	CLA	CHB-C4A-NA	2.72	128.27	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BQ	601	CHL	C1-C2-C3	-2.72	121.34	126.04
31	D	403	PL9	C22-C23-C24	-2.72	121.11	127.66
24	BQ	610	CLA	C1-C2-C3	-2.72	121.34	126.04
24	BV	603	CLA	C3B-C4B-NB	-2.72	107.99	110.52
26	7	319	NEX	C28-C29-C30	2.72	123.11	118.94
23	g	607	CHL	C1-C2-C3	-2.72	121.34	126.04
29	k	101	BCR	C33-C5-C6	-2.72	121.47	124.53
23	8	305	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
24	v	607	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	BB	310	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
23	Ba	309	CHL	CHC-C4B-NB	-2.72	121.38	124.26
23	AA	310	CHL	C3B-C4B-NB	2.72	113.04	110.52
24	v	615	CLA	C3B-C4B-NB	-2.72	107.99	110.52
29	K	102	BCR	C27-C26-C25	2.72	126.68	122.73
24	y	315	CLA	C3B-C4B-NB	-2.72	108.00	110.52
24	BJ	612	CLA	C3B-C4B-NB	-2.72	108.00	110.52
24	A2	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
24	6	612	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
24	6	613	CLA	CAA-CBA-CGA	-2.72	105.32	113.25
23	BJ	609	CHL	CMB-C2B-C1B	2.72	129.50	125.37
24	b	617	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	S	606	CHL	CHB-C4A-NA	2.71	128.27	124.51
24	N	612	CLA	CHB-C4A-NA	2.71	128.27	124.51
23	g	607	CHL	O2A-CGA-CBA	2.71	120.43	111.91
23	Ba	310	CHL	C3D-C4D-ND	2.71	114.63	110.24
23	Au	606	CHL	CMB-C2B-C1B	2.71	129.50	125.37
24	N	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	b	602	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	g	612	CLA	C3B-C4B-NB	-2.71	108.00	110.52
23	Au	606	CHL	C1D-ND-C4D	-2.71	104.41	106.33
23	BV	606	CHL	C6-C5-C3	-2.71	110.18	114.62
23	n	605	CHL	O2A-CGA-CBA	2.71	120.42	111.91
23	Ba	310	CHL	C4-C3-C5	2.71	119.84	115.27
24	Ba	314	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	7	308	CHL	CHB-C4A-NA	2.71	128.26	124.51
26	AA	319	NEX	C28-C29-C30	2.71	123.10	118.94
24	r	609	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	Ba	317	LUT	C15-C35-C34	2.71	129.03	123.47
23	Ba	310	CHL	C6-C5-C3	-2.71	110.19	114.62
23	9	608	CHL	C1D-ND-C4D	-2.71	104.41	106.33
31	BG	403	PL9	C7-C8-C9	-2.71	122.28	126.79
23	BJ	607	CHL	O2A-CGA-CBA	2.71	120.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	g	601	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
24	BE	611	CLA	CBC-CAC-C3C	2.71	119.90	112.43
23	S	607	CHL	CMD-C2D-C3D	-2.71	121.38	127.61
24	9	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	BQ	604	CLA	C3B-C4B-NB	-2.71	108.00	110.52
33	f	102	HEM	C4D-ND-C1D	2.71	107.87	105.07
24	5	610	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	0	606	CHL	CMB-C2B-C1B	2.71	129.50	125.37
38	R	408	PHO	O1D-CGD-CBD	2.71	129.25	124.74
24	b	612	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	BF	511	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	n	601	CHL	C1-C2-C3	-2.71	121.36	126.04
24	S	610	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	7	306	CHL	C2D-C1D-ND	2.71	112.10	110.10
23	8	307	CHL	C1D-ND-C4D	-2.71	104.41	106.33
25	A2	615	LUT	C35-C15-C14	2.71	129.02	123.47
27	6	617	LHG	O8-C23-C24	2.71	120.41	111.91
23	7	308	CHL	C1-C2-C3	-2.71	121.36	126.04
23	AB	305	CHL	CMD-C2D-C3D	-2.71	121.38	127.61
33	BI	102	HEM	C4D-ND-C1D	2.71	107.87	105.07
23	BV	601	CHL	C3B-C4B-NB	2.71	113.03	110.52
24	BE	603	CLA	C3B-C4B-NB	-2.71	108.00	110.52
23	BV	601	CHL	CHC-C4B-NB	-2.71	121.39	124.26
27	Az	102	LHG	O8-C23-C24	2.71	120.40	111.91
23	5	605	CHL	C1C-C2C-C3C	-2.71	104.97	107.11
23	S	605	CHL	CMD-C2D-C3D	-2.71	121.39	127.61
23	G	605	CHL	CAC-C3C-C4C	2.71	128.32	124.81
34	BF	518	DGD	CDB-CCB-CBB	-2.71	100.69	114.42
23	6	606	CHL	O1D-CGD-CBD	-2.71	118.95	124.48
24	g	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	BE	615	CLA	C1-C2-C3	-2.71	121.36	126.04
23	7	302	CHL	CMD-C2D-C3D	-2.71	121.39	127.61
32	BO	101	SQD	O48-C23-C24	2.70	120.40	111.91
29	8	313	BCR	C11-C10-C9	-2.70	123.45	127.31
32	A	413	SQD	O8-S-C6	2.70	110.05	105.74
29	B	619	BCR	C33-C5-C6	-2.70	121.49	124.53
29	Ay	102	BCR	C33-C5-C6	-2.70	121.49	124.53
23	BQ	605	CHL	O2A-CGA-CBA	2.70	120.39	111.91
24	6	611	CLA	C3B-C4B-NB	-2.70	108.01	110.52
23	9	607	CHL	CHB-C4A-NA	2.70	128.25	124.51
24	BF	506	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	Ba	307	CHL	CMD-C2D-C3D	-2.70	121.40	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	405	LMG	O6-C1-O1	-2.70	103.57	109.97
29	AB	313	BCR	C33-C5-C6	-2.70	121.49	124.53
24	C	508	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	A6	604	CLA	C3B-C4B-NB	-2.70	108.01	110.52
23	Au	605	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
25	Ba	316	LUT	C35-C15-C14	2.70	129.01	123.47
24	N	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	BV	604	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	g	616	LUT	C15-C35-C34	2.70	129.01	123.47
24	D	402	CLA	CHB-C4A-NA	2.70	128.25	124.51
29	v	622	BCR	C33-C5-C6	-2.70	121.50	124.53
23	y	309	CHL	CHC-C4B-NB	-2.70	121.40	124.26
24	c	511	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	v	609	CLA	C3B-C4B-NB	-2.70	108.01	110.52
25	N	615	LUT	C35-C15-C14	2.70	129.00	123.47
23	9	609	CHL	CMB-C2B-C1B	2.70	129.48	125.37
24	v	601	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	9	611	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	2	407	LMG	O6-C1-O1	-2.70	103.58	109.97
24	y	304	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	G	608	CHL	OMC-CMC-C2C	-2.70	119.59	125.69
24	A2	604	CLA	C1-C2-C3	-2.70	122.39	126.75
24	BE	614	CLA	C3B-C4B-NB	-2.70	108.01	110.52
29	BK	101	BCR	C27-C26-C25	2.70	126.65	122.73
34	c	517	DGD	CDB-CCB-CBB	-2.70	100.73	114.42
34	BF	517	DGD	O5D-C6D-C5D	-2.70	104.06	109.05
23	BJ	607	CHL	C1-C2-C3	-2.70	121.38	126.04
23	n	601	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
24	b	617	CLA	CHB-C4A-NA	2.70	128.24	124.51
32	l	101	SQD	O48-C23-C24	2.70	120.37	111.91
23	G	601	CHL	C4-C3-C5	2.70	119.81	115.27
23	G	608	CHL	C1D-ND-C4D	-2.70	104.42	106.33
24	A	407	CLA	C1-C2-C3	-2.70	122.39	126.75
24	A6	604	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	Au	609	CHL	C1-C2-C3	-2.69	121.38	126.04
24	BE	605	CLA	C1-C2-C3	-2.69	121.38	126.04
23	BQ	608	CHL	CHC-C4B-NB	-2.69	121.40	124.26
24	BE	612	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	c	505	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	v	612	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	BU	605	CHL	C4-C3-C5	2.69	119.80	115.27
25	N	616	LUT	C12-C13-C14	2.69	123.08	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	610	CLA	C2D-C1D-ND	-2.69	108.12	110.10
23	r	607	CHL	O2D-CGD-O1D	-2.69	118.57	123.84
23	s	606	CHL	O2A-CGA-CBA	2.69	120.36	111.91
23	7	308	CHL	O2A-CGA-CBA	2.69	120.36	111.91
24	r	608	CLA	CHB-C4A-NA	2.69	128.24	124.51
24	Aw	102	CLA	CHB-C4A-NA	2.69	128.24	124.51
24	A2	603	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	0	601	CHL	C1-C2-C3	-2.69	121.39	126.04
24	BE	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	d	402	CLA	C3B-C4B-NB	-2.69	108.02	110.52
23	N	609	CHL	C1D-ND-C4D	-2.69	104.42	106.33
23	A6	605	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
31	d	403	PL9	C7-C8-C9	-2.69	122.31	126.79
23	BU	605	CHL	CHB-C4A-NA	2.69	128.23	124.51
24	g	610	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	BF	512	CLA	C3B-C4B-NB	-2.69	108.02	110.52
23	AA	310	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
23	s	601	CHL	CMB-C2B-C1B	2.69	129.47	125.37
23	BB	309	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
24	A	407	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	BE	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	BF	502	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	B	601	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	BB	305	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	G	604	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	A6	607	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
24	C	510	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	C	508	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	2	403	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	A6	606	CHL	O2A-CGA-CBA	2.69	120.34	111.91
38	a	409	PHO	O1D-CGD-CBD	2.69	129.21	124.74
24	n	604	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	D	406	SQD	O48-C23-C24	2.69	120.34	111.91
24	r	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	9	615	LUT	C32-C33-C34	2.69	123.06	118.94
23	5	609	CHL	CAC-C3C-C4C	2.69	128.29	124.81
24	c	508	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
23	9	605	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
29	v	619	BCR	C33-C5-C6	-2.68	121.51	124.53
23	S	606	CHL	O2A-CGA-CBA	2.68	120.33	111.91
29	B	618	BCR	C15-C16-C17	-2.68	117.97	123.47
24	B	602	CLA	CHB-C4A-NA	2.68	128.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	617	NEX	C28-C29-C30	2.68	123.06	118.94
24	N	603	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	b	609	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	s	611	CLA	CHB-C4A-NA	2.68	128.22	124.51
38	R	408	PHO	C1C-C2C-C3C	-2.68	106.38	108.61
27	L	102	LHG	O8-C23-C24	2.68	120.33	111.91
24	8	308	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	AA	316	LUT	C32-C33-C34	2.68	123.06	118.94
24	Y	313	CLA	C3B-C4B-NB	-2.68	108.03	110.52
24	Au	603	CLA	C3B-C4B-NB	-2.68	108.03	110.52
23	g	609	CHL	CHD-C1D-C2D	2.68	131.10	125.48
23	5	607	CHL	O2D-CGD-O1D	-2.68	118.59	123.84
24	Y	304	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	A2	605	CHL	CHB-C4A-NA	2.68	128.22	124.51
24	y	305	CLA	C1-C2-C3	-2.68	122.41	126.75
24	BF	506	CLA	C3B-C4B-NB	-2.68	108.03	110.52
23	6	606	CHL	CMB-C2B-C1B	2.68	129.45	125.37
24	1	507	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	C	507	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	BE	617	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	AB	306	CHL	C3B-C4B-NB	2.68	113.00	110.52
24	1	503	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	5	616	LUT	C32-C33-C34	2.68	123.05	118.94
24	C	510	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	6	601	CHL	O2A-CGA-CBA	2.68	120.32	111.91
24	BQ	604	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	N	609	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
23	N	606	CHL	C3B-C4B-NB	2.68	113.00	110.52
27	N	618	LHG	O8-C23-C24	2.68	120.31	111.91
23	AA	302	CHL	CMB-C2B-C1B	2.68	129.45	125.37
25	5	615	LUT	C15-C35-C34	2.68	128.96	123.47
24	BE	602	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	BB	317	LUT	C12-C13-C14	2.68	123.05	118.94
23	r	605	CHL	C4-C3-C5	2.68	119.77	115.27
23	9	607	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
24	0	610	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
23	AA	306	CHL	C2D-C1D-ND	2.68	112.08	110.10
23	N	605	CHL	O2A-CGA-CBA	2.68	120.30	111.91
29	AB	313	BCR	C24-C23-C22	-2.67	122.19	126.23
23	BJ	606	CHL	CHB-C4A-NA	2.67	128.21	124.51
24	I	102	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	BV	606	CHL	O2A-CGA-CBA	2.67	120.30	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	609	CHL	CHD-C1D-C2D	2.67	131.09	125.48
24	v	613	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
24	BD	406	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	Y	302	CHL	C1C-C2C-C3C	-2.67	104.99	107.11
30	B	620	LMG	O6-C1-O1	-2.67	103.64	109.97
24	Y	303	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	B	612	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	BJ	616	LUT	C15-C35-C34	2.67	128.95	123.47
23	N	607	CHL	O2A-CGA-CBA	2.67	120.30	111.91
23	Ba	302	CHL	C6-C5-C3	-2.67	110.25	114.62
24	7	303	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	0	604	CLA	C3B-C4B-NB	-2.67	108.04	110.52
24	BB	303	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	y	307	CHL	CMD-C2D-C3D	-2.67	121.47	127.61
38	A	409	PHO	O1D-CGD-CBD	2.67	129.19	124.74
24	BB	315	CLA	C3B-C4B-NB	-2.67	108.04	110.52
23	r	605	CHL	CHB-C4A-NA	2.67	128.20	124.51
23	A2	607	CHL	O2A-CGA-CBA	2.67	120.28	111.91
25	7	317	LUT	C12-C13-C14	2.67	123.04	118.94
24	b	613	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	n	611	CLA	C3B-C4B-NB	-2.67	108.04	110.52
24	R	406	CLA	C3B-C4B-NB	-2.67	108.04	110.52
25	y	316	LUT	C12-C13-C14	2.67	123.03	118.94
23	BQ	605	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
25	s	614	LUT	C39-C29-C28	2.67	122.28	118.08
24	S	611	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	0	601	CHL	CMB-C2B-C1B	2.66	129.43	125.37
24	v	616	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
24	0	603	CLA	C3B-C4B-NB	-2.66	108.04	110.52
24	BV	602	CLA	C3B-C4B-NB	-2.66	108.04	110.52
24	N	604	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	BF	513	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	Au	601	CHL	C4-C3-C5	2.66	119.75	115.27
27	A2	618	LHG	O8-C23-C24	2.66	120.27	111.91
23	y	310	CHL	C3D-C4D-ND	2.66	114.54	110.24
23	AB	304	CHL	C3D-C4D-ND	2.66	114.54	110.24
23	8	305	CHL	C1D-ND-C4D	-2.66	104.44	106.33
23	s	601	CHL	C3B-C4B-NB	2.66	112.98	110.52
24	8	309	CLA	C3B-C4B-NB	-2.66	108.05	110.52
23	BB	306	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
24	S	604	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	A2	604	CLA	CHB-C4A-NA	2.66	128.19	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	Ba	315	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	b	606	CLA	C3B-C4B-NB	-2.66	108.05	110.52
23	AB	305	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
29	BF	516	BCR	C27-C26-C25	2.66	126.59	122.73
24	b	611	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	BE	606	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	BQ	611	CLA	C3B-C4B-NB	-2.66	108.05	110.52
23	A2	601	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
24	B	614	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	8	306	CHL	C3B-C4B-NB	2.66	112.98	110.52
24	1	510	CLA	C3B-C4B-NB	-2.66	108.05	110.52
23	5	609	CHL	C3D-C4D-ND	2.66	114.54	110.24
24	y	315	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	A6	616	NEX	C28-C29-C30	2.66	123.02	118.94
24	C	504	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	Ba	304	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
32	BO	102	SQD	O48-C23-C24	2.66	120.25	111.91
24	BE	607	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	1	508	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	s	601	CHL	OMC-CMC-C2C	-2.66	119.68	125.69
23	A2	608	CHL	OMC-CMC-C2C	-2.66	119.68	125.69
23	g	608	CHL	C1-C2-C3	-2.66	121.45	126.04
24	0	610	CLA	CHB-C1B-NB	2.66	127.07	124.26
24	d	401	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	1	507	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	y	313	CLA	CHB-C4A-NA	2.66	128.18	124.51
23	7	302	CHL	CMB-C2B-C1B	2.66	129.41	125.37
24	y	314	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
23	5	608	CHL	C1D-ND-C4D	-2.65	104.45	106.33
25	n	616	LUT	C15-C35-C34	2.65	128.91	123.47
23	AA	308	CHL	O2A-C1-C2	-2.65	101.66	108.64
24	n	604	CLA	C3B-C4B-NB	-2.65	108.05	110.52
25	G	615	LUT	C8-C9-C10	2.65	123.01	118.94
23	0	609	CHL	C3D-C4D-ND	2.65	114.53	110.24
23	s	606	CHL	C6-C5-C3	-2.65	110.28	114.62
24	A	405	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	BU	605	CHL	C4A-NA-C1A	2.65	107.90	106.71
24	a	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	Av	101	BCR	C33-C5-C6	-2.65	121.55	124.53
24	BG	402	CLA	C3B-C4B-NB	-2.65	108.06	110.52
24	BJ	613	CLA	C3B-C4B-NB	-2.65	108.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	G	601	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
24	A2	611	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	A6	611	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	e	601	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
24	N	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	C	511	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	n	608	CHL	CHC-C4B-NB	-2.65	121.45	124.26
23	y	307	CHL	C3D-C4D-ND	2.65	114.52	110.24
24	7	311	CLA	CHB-C4A-NA	2.65	128.17	124.51
24	s	604	CLA	CHB-C4A-NA	2.65	128.17	124.51
29	b	618	BCR	C15-C14-C13	-2.65	123.53	127.31
24	BU	608	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	I	101	LMG	O2-C2-C1	-2.65	103.62	110.05
23	BQ	609	CHL	CMB-C2B-C1B	2.65	129.40	125.37
23	G	605	CHL	CMD-C2D-C3D	-2.65	121.53	127.61
23	n	609	CHL	C1D-ND-C4D	-2.65	104.45	106.33
24	B	616	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	6	609	CHL	C3B-C4B-NB	2.65	112.97	110.52
24	Ba	314	CLA	C3B-C4B-NB	-2.65	108.06	110.52
24	1	504	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	A6	607	CHL	C3D-C4D-ND	2.65	114.52	110.24
24	b	612	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
23	BU	607	CHL	CMD-C2D-C3D	-2.65	121.53	127.61
23	n	607	CHL	O2A-CGA-CBA	2.65	120.21	111.91
27	A0	202	LHG	O8-C23-C24	2.65	120.21	111.91
24	G	614	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	n	609	CHL	CHC-C4B-NB	-2.64	121.46	124.26
29	BF	516	BCR	C15-C14-C13	-2.64	123.54	127.31
24	BV	611	CLA	CHB-C4A-NA	2.64	128.17	124.51
29	c	515	BCR	C15-C14-C13	-2.64	123.54	127.31
23	BJ	605	CHL	CHB-C4A-NA	2.64	128.17	124.51
24	AA	303	CLA	CAC-C3C-C4C	2.64	128.24	124.81
24	b	614	CLA	CHB-C4A-NA	2.64	128.17	124.51
24	R	409	CLA	CHB-C4A-NA	2.64	128.17	124.51
23	G	607	CHL	CHB-C4A-NA	2.64	128.16	124.51
29	B	619	BCR	C24-C23-C22	-2.64	122.25	126.23
29	Bb	101	BCR	C24-C23-C22	-2.64	122.25	126.23
24	D	401	CLA	C3B-C4B-NB	-2.64	108.07	110.52
24	AB	309	CLA	C3B-C4B-NB	-2.64	108.07	110.52
24	c	513	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	A6	601	CHL	OMC-CMC-C2C	-2.64	119.72	125.69
24	n	610	CLA	C2A-C3A-C4A	2.64	106.13	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	303	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	v	616	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	BU	609	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	BQ	608	CHL	C4A-NA-C1A	2.64	107.89	106.71
23	5	607	CHL	CMD-C2D-C3D	-2.64	121.55	127.61
23	BB	310	CHL	O2A-CGA-CBA	2.64	120.19	111.91
23	6	601	CHL	CMB-C2B-C1B	2.64	129.39	125.37
23	Y	310	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
23	BQ	601	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
24	6	612	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	S	604	CLA	C1-C2-C3	-2.64	122.49	126.75
23	BB	302	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
29	A	411	BCR	C24-C23-C22	-2.64	122.25	126.23
24	B	609	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
24	BF	513	CLA	C3B-C4B-NB	-2.64	108.07	110.52
23	A6	601	CHL	CHC-C4B-NB	-2.64	121.47	124.26
23	AB	306	CHL	C3D-C4D-ND	2.63	114.50	110.24
25	n	615	LUT	C32-C33-C34	2.63	122.98	118.94
23	N	608	CHL	OMC-CMC-C2C	-2.63	119.73	125.69
24	S	610	CLA	CHB-C4A-NA	2.63	128.16	124.51
24	g	613	CLA	C3B-C4B-NB	-2.63	108.07	110.52
23	n	601	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
24	r	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	S	611	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	BE	611	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	y	308	CHL	O2A-CGA-CBA	2.63	120.17	111.91
32	l	102	SQD	O48-C23-C24	2.63	120.17	111.91
24	BU	609	CLA	C3B-C4B-NB	-2.63	108.07	110.52
23	BQ	607	CHL	O2A-CGA-CBA	2.63	120.17	111.91
24	R	404	CLA	C3B-C4B-NB	-2.63	108.07	110.52
24	7	315	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	C	514	BCR	C27-C26-C25	2.63	126.55	122.73
24	c	513	CLA	C1-C2-C3	-2.63	121.49	126.04
23	BQ	601	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
24	BJ	610	CLA	C3B-C4B-NB	-2.63	108.07	110.52
23	Ba	306	CHL	O2A-CGA-CBA	2.63	120.16	111.91
26	S	616	NEX	C28-C29-C30	2.63	122.98	118.94
25	A6	614	LUT	C39-C29-C28	2.63	122.22	118.08
23	AB	305	CHL	C1D-ND-C4D	-2.63	104.47	106.33
24	BG	401	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	7	315	CLA	C3B-C4B-NB	-2.63	108.08	110.52
24	BE	610	CLA	C3B-C4B-NB	-2.63	108.08	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	601	CHL	CHC-C4B-NB	-2.63	121.47	124.26
23	8	306	CHL	C3D-C4D-ND	2.63	114.49	110.24
24	Y	315	CLA	C3B-C4B-NB	-2.63	108.08	110.52
24	A6	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	Au	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
24	c	514	CLA	C3B-C4B-NB	-2.63	108.08	110.52
25	AB	311	LUT	C8-C9-C10	2.63	122.97	118.94
23	AA	310	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
23	Ba	308	CHL	O2A-CGA-CBA	2.63	120.15	111.91
25	BQ	616	LUT	C15-C35-C34	2.63	128.85	123.47
24	g	614	CLA	C3B-C4B-NB	-2.63	108.08	110.52
25	BQ	615	LUT	C32-C33-C34	2.63	122.97	118.94
24	r	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	B	623	BCR	C33-C5-C6	-2.63	121.58	124.53
34	BF	517	DGD	C3G-C2G-C1G	-2.63	105.58	111.79
29	1	514	BCR	C27-C26-C25	2.62	126.54	122.73
23	N	601	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
25	S	614	LUT	C39-C29-C28	2.62	122.21	118.08
24	6	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	G	606	CHL	C1D-ND-C4D	-2.62	104.47	106.33
23	BJ	609	CHL	C3B-C4B-NB	2.62	112.95	110.52
24	C	503	CLA	C3B-C4B-NB	-2.62	108.08	110.52
23	y	306	CHL	O2A-CGA-CBA	2.62	120.14	111.91
23	BQ	606	CHL	C3D-C4D-ND	2.62	114.48	110.24
25	BU	615	LUT	C32-C33-C34	2.62	122.97	118.94
24	1	509	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	BF	508	CLA	CHB-C4A-NA	2.62	128.14	124.51
27	y	319	LHG	O8-C23-C24	2.62	120.14	111.91
24	N	613	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	BJ	603	CLA	C3B-C4B-NB	-2.62	108.08	110.52
23	S	601	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
24	c	513	CLA	C3B-C4B-NB	-2.62	108.08	110.52
29	z	101	BCR	C15-C14-C13	-2.62	123.57	127.31
23	6	608	CHL	CHC-C4B-NB	-2.62	121.48	124.26
24	Ba	305	CLA	C1-C2-C3	-2.62	122.51	126.75
24	y	314	CLA	C1-C2-C3	-2.62	121.51	126.04
24	B	607	CLA	CHB-C4A-NA	2.62	128.14	124.51
32	d	406	SQD	O48-C23-C24	2.62	120.13	111.91
24	v	611	CLA	O2D-CGD-CBD	2.62	115.92	111.27
29	C	515	BCR	C7-C8-C9	-2.62	122.28	126.23
23	BJ	607	CHL	C4-C3-C5	2.62	119.68	115.27
23	8	304	CHL	C1C-C2C-C3C	-2.62	105.03	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	606	CHL	C1D-ND-C4D	-2.62	104.47	106.33
24	c	508	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	c	511	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	BB	316	LUT	C32-C33-C34	2.62	122.96	118.94
23	Y	310	CHL	O2A-CGA-CBA	2.62	120.13	111.91
23	0	608	CHL	OMC-CMC-C2C	-2.62	119.77	125.69
24	BE	615	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	BJ	611	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	Ba	303	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	Ba	313	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	G	616	LUT	C12-C13-C14	2.62	122.96	118.94
34	C	516	DGD	O5D-C6D-C5D	-2.62	104.20	109.05
23	BJ	608	CHL	C1-C2-C3	-2.62	121.52	126.04
23	S	601	CHL	CHC-C4B-NB	-2.62	121.49	124.26
23	Y	307	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
24	y	303	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	BU	614	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	Au	601	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
34	c	516	DGD	O5D-C6D-C5D	-2.62	104.21	109.05
24	N	612	CLA	C3B-C4B-NB	-2.62	108.09	110.52
23	g	607	CHL	C4-C3-C5	2.62	119.67	115.27
24	A	406	CLA	CHB-C4A-NA	2.61	128.13	124.51
24	AA	304	CLA	CHB-C4A-NA	2.61	128.13	124.51
29	C	515	BCR	C27-C26-C25	2.61	126.53	122.73
24	9	602	CLA	CHB-C1B-NB	2.61	127.02	124.26
23	5	609	CHL	O2D-CGD-O1D	-2.61	118.73	123.84
29	BE	618	BCR	C11-C10-C9	-2.61	123.58	127.31
24	c	508	CLA	C3B-C4B-NB	-2.61	108.09	110.52
24	B	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	Au	616	LUT	C12-C13-C14	2.61	122.95	118.94
38	A	409	PHO	C1C-C2C-C3C	-2.61	106.44	108.61
23	y	308	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
24	BB	304	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	R	410	BCR	C24-C23-C22	-2.61	122.29	126.23
23	g	606	CHL	C1D-ND-C4D	-2.61	104.48	106.33
24	g	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
27	B	622	LHG	O8-C23-C24	2.61	120.10	111.91
24	B	610	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	s	606	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
23	Ba	310	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
27	BU	617	LHG	C11-C10-C9	-2.61	101.18	114.42
24	g	611	CLA	CHB-C4A-NA	2.61	128.12	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	z	101	BCR	C27-C26-C25	2.61	126.52	122.73
23	Y	306	CHL	CHC-C4B-NB	-2.61	121.50	124.26
27	r	618	LHG	C11-C10-C9	-2.61	101.18	114.42
25	BV	614	LUT	C39-C29-C28	2.61	122.19	118.08
24	g	610	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	B	611	CLA	O2D-CGD-CBD	2.61	115.90	111.27
27	BE	624	LHG	O8-C23-C24	2.61	120.09	111.91
24	b	611	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	9	610	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	BJ	601	CHL	O2A-CGA-CBA	2.61	120.09	111.91
24	r	601	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	Ba	318	NEX	C28-C29-C30	2.61	122.94	118.94
23	BJ	605	CHL	C1C-C2C-C3C	-2.61	105.05	107.11
24	Ba	314	CLA	C1-C2-C3	-2.61	121.53	126.04
24	c	507	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	v	602	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	BU	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	BB	307	CHL	CMD-C2D-C3D	-2.61	121.62	127.61
32	D	406	SQD	O5-C5-C4	2.61	114.43	109.69
27	B	621	LHG	O8-C23-C24	2.61	120.09	111.91
23	Y	310	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
24	b	605	CLA	C1-C2-C3	-2.61	121.54	126.04
24	BB	305	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	AA	314	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	b	615	CLA	C1-C2-C3	-2.61	121.54	126.04
23	Ba	307	CHL	C3D-C4D-ND	2.61	114.45	110.24
24	c	506	CLA	CHB-C4A-NA	2.60	128.11	124.51
27	v	621	LHG	O8-C23-C24	2.60	120.08	111.91
24	BJ	611	CLA	C3B-C4B-NB	-2.60	108.10	110.52
25	r	615	LUT	C8-C9-C10	2.60	122.94	118.94
24	Au	614	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	b	601	BCR	C24-C23-C22	-2.60	122.30	126.23
23	8	305	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
24	9	612	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	AB	307	CHL	CHC-C4B-NB	-2.60	121.50	124.26
29	R	410	BCR	C33-C5-C6	-2.60	121.61	124.53
24	6	604	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	1	515	BCR	C7-C8-C9	-2.60	122.30	126.23
24	A2	614	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	Ba	302	CHL	C4-C3-C5	2.60	119.65	115.27
24	A	410	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	n	610	CLA	C1-C2-C3	-2.60	121.54	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	607	CHL	C1D-ND-C4D	-2.60	104.49	106.33
24	b	607	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	C	519	LMG	O6-C1-O1	-2.60	103.81	109.97
24	s	602	CLA	C3B-C4B-NB	-2.60	108.10	110.52
23	0	608	CHL	CHC-C4B-NB	-2.60	121.50	124.26
23	AA	306	CHL	CHC-C4B-NB	-2.60	121.50	124.26
34	a	413	DGD	C3G-C2G-C1G	-2.60	105.64	111.79
29	8	313	BCR	C24-C23-C22	-2.60	122.31	126.23
24	v	616	CLA	C3B-C4B-NB	-2.60	108.10	110.52
27	Ba	319	LHG	O8-C23-C24	2.60	120.06	111.91
27	W	201	LHG	O8-C23-C24	2.60	120.06	111.91
24	BE	604	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	R	405	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	0	607	CHL	C4-C3-C5	2.60	119.64	115.27
24	R	405	CLA	C3B-C4B-NB	-2.60	108.10	110.52
24	N	614	CLA	CHB-C4A-NA	2.60	128.10	124.51
24	Au	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
24	Au	612	CLA	CHB-C4A-NA	2.60	128.10	124.51
32	2	408	SQD	O48-C23-C24	2.60	120.06	111.91
29	BE	618	BCR	C15-C14-C13	-2.60	123.60	127.31
34	1	516	DGD	O5D-C6D-C5D	-2.60	104.24	109.05
25	r	615	LUT	C32-C33-C34	2.60	122.93	118.94
24	B	605	CLA	C3B-C4B-NB	-2.60	108.11	110.52
23	Y	309	CHL	CHC-C4B-NB	-2.60	121.51	124.26
23	BB	309	CHL	CHC-C4B-NB	-2.60	121.51	124.26
24	A6	611	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
24	G	602	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	N	606	CHL	C1D-ND-C4D	-2.60	104.49	106.33
24	c	503	CLA	C3B-C4B-NB	-2.60	108.11	110.52
24	BV	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
27	2	405	LHG	O8-C23-C24	2.60	120.05	111.91
24	B	616	CLA	CHB-C4A-NA	2.59	128.10	124.51
29	Bb	101	BCR	C15-C14-C13	-2.59	123.61	127.31
23	g	601	CHL	O2A-CGA-CBA	2.59	120.05	111.91
29	BF	515	BCR	C27-C26-C25	2.59	126.50	122.73
24	AA	315	CLA	C3B-C4B-NB	-2.59	108.11	110.52
23	5	607	CHL	C1D-ND-C4D	-2.59	104.49	106.33
24	7	314	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
24	BF	512	CLA	CHB-C4A-NA	2.59	128.10	124.51
24	9	604	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
26	r	617	NEX	C28-C29-C30	2.59	122.92	118.94
23	0	601	CHL	O2A-CGA-CBA	2.59	120.05	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	606	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
24	s	603	CLA	CHB-C4A-NA	2.59	128.10	124.51
23	0	601	CHL	C6-C5-C3	-2.59	110.38	114.62
24	2	402	CLA	C3B-C4B-NB	-2.59	108.11	110.52
38	BD	409	PHO	O2D-CGD-O1D	-2.59	118.77	123.84
25	BJ	616	LUT	C11-C12-C13	2.59	133.69	126.42
24	r	609	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	6	610	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
23	BV	606	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
23	6	607	CHL	C4-C3-C5	2.59	119.63	115.27
24	b	604	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	r	603	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	A2	613	CLA	C3B-C4B-NB	-2.59	108.11	110.52
23	BJ	606	CHL	C1D-ND-C4D	-2.59	104.50	106.33
24	Y	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	BJ	610	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	Ba	313	CLA	C3B-C4B-NB	-2.59	108.11	110.52
23	A6	605	CHL	CHB-C4A-NA	2.59	128.09	124.51
24	BE	608	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	BJ	610	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
24	R	404	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	y	313	CLA	C3B-C4B-NB	-2.59	108.11	110.52
24	v	607	CLA	C3B-C4B-NB	-2.59	108.11	110.52
34	1	517	DGD	O5D-C6D-C5D	-2.59	104.26	109.05
34	1	516	DGD	C3G-C2G-C1G	-2.59	105.67	111.79
24	y	304	CLA	CHB-C4A-NA	2.59	128.09	124.51
34	C	518	DGD	C3G-C2G-C1G	-2.59	105.67	111.79
23	AA	306	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
27	b	624	LHG	C11-C10-C9	-2.59	101.29	114.42
26	y	318	NEX	C28-C29-C30	2.59	122.91	118.94
31	2	404	PL9	O1-C4-C3	-2.59	117.87	120.72
24	BV	602	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
24	v	602	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	BU	610	CLA	CHB-C4A-NA	2.58	128.09	124.51
29	H	101	BCR	C33-C5-C6	-2.58	121.63	124.53
29	1	515	BCR	C27-C26-C25	2.58	126.48	122.73
34	BD	413	DGD	C3G-C2G-C1G	-2.58	105.68	111.79
29	BE	619	BCR	C15-C16-C17	-2.58	118.18	123.47
23	N	607	CHL	CHB-C4A-NA	2.58	128.09	124.51
24	AA	315	CLA	CHB-C4A-NA	2.58	128.09	124.51
29	BE	618	BCR	C38-C26-C27	-2.58	108.65	113.62
23	6	601	CHL	CHC-C4B-NB	-2.58	121.52	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
24	8	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	c	503	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	AB	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	C	510	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	Au	614	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	1	511	CLA	C3B-C4B-NB	-2.58	108.12	110.52
27	BB	319	LHG	O8-C23-C24	2.58	120.01	111.91
23	AB	304	CHL	C1C-C2C-C3C	-2.58	105.07	107.11
24	BU	601	CLA	CHB-C1B-NB	2.58	126.99	124.26
23	N	605	CHL	CHB-C4A-NA	2.58	128.08	124.51
24	BE	603	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	b	608	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	v	611	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	BU	609	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
25	8	311	LUT	C15-C35-C34	2.58	128.76	123.47
24	s	611	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	v	614	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	BE	601	BCR	C24-C23-C22	-2.58	122.34	126.23
29	v	618	BCR	C27-C26-C25	2.58	126.47	122.73
23	g	609	CHL	C3B-C4B-NB	2.58	112.91	110.52
24	BU	611	CLA	CHB-C4A-NA	2.58	128.07	124.51
32	A1	101	SQD	O48-C23-C24	2.58	119.99	111.91
24	b	610	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	y	314	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	C	509	CLA	CHB-C4A-NA	2.58	128.07	124.51
25	6	615	LUT	C35-C15-C14	2.58	128.75	123.47
24	S	611	CLA	C3B-C4B-NB	-2.58	108.13	110.52
24	r	611	CLA	CHB-C4A-NA	2.58	128.07	124.51
23	y	309	CHL	C4-C3-C5	2.57	119.60	115.27
23	9	609	CHL	O1D-CGD-CBD	-2.57	119.22	124.48
24	C	511	CLA	CHA-C4D-ND	2.57	137.88	132.50
24	7	304	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	1	519	LMG	O6-C1-O1	-2.57	103.88	109.97
24	BQ	602	CLA	C3B-C4B-NB	-2.57	108.13	110.52
24	1	511	CLA	CHB-C4A-NA	2.57	128.07	124.51
32	L	103	SQD	O48-C23-C24	2.57	119.98	111.91
24	A6	612	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	BV	612	CLA	C3B-C4B-NB	-2.57	108.13	110.52
23	g	605	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
23	y	306	CHL	C1D-ND-C4D	-2.57	104.51	106.33
24	BF	503	CLA	CHB-C4A-NA	2.57	128.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A2	616	LUT	C32-C33-C34	2.57	122.89	118.94
24	A2	610	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
34	1	518	DGD	C3G-C2G-C1G	-2.57	105.71	111.79
29	A	411	BCR	C33-C5-C6	-2.57	121.64	124.53
24	BG	402	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	G	608	CHL	C1-C2-C3	-2.57	121.60	126.04
23	Ba	308	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
23	BH	601	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
26	s	616	NEX	C28-C29-C30	2.57	122.89	118.94
23	g	606	CHL	CHB-C4A-NA	2.57	128.07	124.51
27	5	618	LHG	O8-C23-C24	2.57	119.97	111.91
23	A2	607	CHL	CHB-C4A-NA	2.57	128.06	124.51
24	G	614	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	r	613	CHL	C1C-C2C-C3C	-2.57	105.08	107.11
23	7	310	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
23	7	306	CHL	CHC-C4B-NB	-2.57	121.54	124.26
34	R	401	DGD	C3G-C2G-C1G	-2.57	105.71	111.79
24	G	603	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	A2	609	CHL	O2A-CGA-CBA	2.57	119.97	111.91
24	BG	401	CLA	C3B-C4B-NB	-2.57	108.13	110.52
24	6	614	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	BQ	603	CLA	CHB-C4A-NA	2.57	128.06	124.51
29	c	515	BCR	C7-C8-C9	-2.57	122.36	126.23
23	BJ	606	CHL	CAA-C2A-C1A	2.57	120.39	111.97
29	b	618	BCR	C30-C25-C26	-2.57	119.00	122.61
24	Y	305	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	b	624	LHG	O8-C23-C24	2.57	119.96	111.91
24	BU	614	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	BU	605	CHL	C2C-C3C-C4C	-2.57	104.66	106.49
24	5	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
30	BE	621	LMG	O1-C7-C8	-2.57	104.71	110.90
23	Ba	309	CHL	C4-C3-C5	2.57	119.59	115.27
23	e	601	CHL	CMD-C2D-C3D	-2.57	121.71	127.61
27	w	201	LHG	O8-C23-C24	2.57	119.96	111.91
24	A6	609	CLA	CHB-C1B-NB	2.57	126.97	124.26
34	C	517	DGD	O5D-C6D-C5D	-2.57	104.30	109.05
24	BF	507	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	n	618	LHG	C11-C10-C9	-2.56	101.40	114.42
27	Y	319	LHG	O8-C23-C24	2.56	119.96	111.91
29	z	102	BCR	C24-C23-C22	-2.56	122.36	126.23
24	BJ	614	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	0	615	LUT	C12-C13-C14	2.56	122.88	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	612	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	6	606	CHL	CMD-C2D-C3D	-2.56	121.72	127.61
24	Au	602	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	b	612	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	C	505	CLA	C3B-C4B-NB	-2.56	108.14	110.52
23	BH	601	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
29	b	619	BCR	C15-C16-C17	-2.56	118.22	123.47
27	D	404	LHG	C11-C10-C9	-2.56	101.42	114.42
24	A	406	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	Ba	305	CLA	C3B-C4B-NB	-2.56	108.14	110.52
23	AB	306	CHL	O2D-CGD-O1D	-2.56	118.83	123.84
24	g	610	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
27	BY	201	LHG	O8-C23-C24	2.56	119.95	111.91
27	0	617	LHG	C11-C10-C9	-2.56	101.42	114.42
27	BQ	618	LHG	C11-C10-C9	-2.56	101.42	114.42
26	BB	320	NEX	C28-C29-C30	2.56	122.87	118.94
34	C	516	DGD	C3G-C2G-C1G	-2.56	105.73	111.79
25	BB	316	LUT	C12-C13-C14	2.56	122.87	118.94
23	s	607	CHL	CHC-C4B-NB	-2.56	121.55	124.26
24	N	610	CLA	C1-C2-C3	-2.56	121.62	126.04
23	N	609	CHL	O2A-CGA-CBA	2.56	119.94	111.91
32	a	412	SQD	O48-C23-C24	2.56	119.94	111.91
24	8	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
23	s	607	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
24	d	402	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	6	605	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
24	C	502	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	b	621	LMG	O1-C7-C8	-2.56	104.73	110.90
24	v	605	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	n	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	C	506	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	BV	607	CHL	CHC-C4B-NB	-2.56	121.55	124.26
29	1	515	BCR	C33-C5-C6	-2.55	121.66	124.53
24	BB	311	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
24	6	603	CLA	C3B-C4B-NB	-2.55	108.14	110.52
24	8	308	CLA	C2D-C1D-ND	-2.55	108.22	110.10
24	G	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	Au	616	LUT	C15-C35-C34	2.55	128.70	123.47
23	r	607	CHL	CMD-C2D-C3D	-2.55	121.74	127.61
24	1	502	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	B	618	BCR	C27-C26-C25	2.55	126.44	122.73
24	B	602	CLA	C3B-C4B-NB	-2.55	108.15	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Au	607	CHL	CHB-C4A-NA	2.55	128.04	124.51
24	Ba	304	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	N	605	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
24	B	607	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	s	612	CLA	C3B-C4B-NB	-2.55	108.15	110.52
38	a	409	PHO	O2D-CGD-O1D	-2.55	118.85	123.84
33	4	102	HEM	C1B-NB-C4B	2.55	107.71	105.07
23	BU	607	CHL	O2A-CGA-CBA	2.55	119.91	111.91
24	0	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	0	605	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
34	A	402	DGD	C3G-C2G-C1G	-2.55	105.76	111.79
23	6	601	CHL	C4-C3-C5	2.55	119.56	115.27
25	s	615	LUT	C39-C29-C28	2.55	122.09	118.08
27	6	617	LHG	C11-C10-C9	-2.55	101.48	114.42
25	Y	316	LUT	C32-C33-C34	2.55	122.85	118.94
24	b	603	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	Au	604	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	5	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
24	v	610	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	Au	616	LUT	C8-C9-C10	2.55	122.85	118.94
23	Ba	306	CHL	C1D-ND-C4D	-2.55	104.53	106.33
23	r	607	CHL	O2A-CGA-CBA	2.55	119.90	111.91
29	BF	515	BCR	C15-C14-C13	-2.55	123.68	127.31
24	8	302	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	G	603	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	G	604	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	y	305	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	n	614	CLA	CHB-C4A-NA	2.55	128.03	124.51
24	A6	602	CLA	C3B-C4B-NB	-2.54	108.15	110.52
23	BH	601	CHL	C2A-C1A-CHA	-2.54	119.41	123.86
24	D	401	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	Y	302	CHL	C2A-C1A-CHA	-2.54	119.41	123.86
29	b	619	BCR	C27-C26-C25	2.54	126.42	122.73
29	F	101	BCR	C24-C23-C22	-2.54	122.39	126.23
23	Y	306	CHL	C1D-ND-C4D	-2.54	104.53	106.33
23	BJ	607	CHL	C2A-C1A-CHA	-2.54	119.41	123.86
23	7	310	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
24	A6	613	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	Au	619	XAT	C12-C13-C14	-2.54	115.04	118.94
24	BF	508	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	c	512	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	g	606	CHL	CAA-C2A-C1A	2.54	120.30	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	BG	406	SQD	O48-C23-C24	2.54	119.88	111.91
24	BV	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	8	306	CHL	CMD-C2D-C3D	-2.54	121.77	127.61
23	BB	306	CHL	C1D-ND-C4D	-2.54	104.53	106.33
29	b	618	BCR	C11-C10-C9	-2.54	123.69	127.31
23	6	606	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
25	Ba	317	LUT	C12-C13-C14	2.54	122.84	118.94
29	v	617	BCR	C11-C10-C9	-2.54	123.69	127.31
29	Ay	102	BCR	C15-C14-C13	-2.54	123.69	127.31
24	B	616	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	BE	608	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	S	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	BB	310	CHL	C1D-ND-C4D	-2.54	104.53	106.33
38	a	409	PHO	CMB-C2B-C3B	2.54	129.43	124.68
24	C	505	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	BF	503	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	BU	602	CLA	C3B-C4B-NB	-2.54	108.16	110.52
25	7	316	LUT	C12-C13-C14	2.54	122.83	118.94
29	BE	620	BCR	C24-C23-C22	-2.54	122.40	126.23
28	G	619	XAT	C12-C13-C14	-2.54	115.05	118.94
25	AA	317	LUT	C39-C29-C28	2.54	122.07	118.08
23	6	609	CHL	CHD-C1D-C2D	2.54	130.80	125.48
32	BD	412	SQD	O48-C23-C24	2.53	119.86	111.91
24	Y	304	CLA	CHB-C4A-NA	2.53	128.02	124.51
24	n	604	CLA	CHB-C4A-NA	2.53	128.02	124.51
24	7	303	CLA	C3B-C4B-NB	-2.53	108.16	110.52
24	AA	311	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	Au	608	CHL	C1-C2-C3	-2.53	121.66	126.04
27	9	618	LHG	O8-C23-C24	2.53	119.86	111.91
23	BB	306	CHL	CHC-C4B-NB	-2.53	121.58	124.26
28	AB	312	XAT	C25-C24-C23	-2.53	107.74	112.75
29	h	101	BCR	C24-C23-C22	-2.53	122.41	126.23
23	g	608	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
24	A	405	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	y	319	LHG	C11-C10-C9	-2.53	101.57	114.42
27	BE	624	LHG	C11-C10-C9	-2.53	101.57	114.42
29	R	410	BCR	C27-C26-C25	2.53	126.41	122.73
27	1	521	LHG	C20-C19-C18	-2.53	101.57	114.42
24	A2	612	CLA	C3B-C4B-NB	-2.53	108.17	110.52
29	BK	101	BCR	C24-C23-C22	-2.53	122.41	126.23
24	b	615	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	1	505	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	S	605	CHL	CHB-C4A-NA	2.53	128.01	124.51
24	7	313	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	g	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	7	306	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
29	BE	619	BCR	C27-C26-C25	2.53	126.40	122.73
31	D	403	PL9	C27-C28-C29	-2.53	121.57	127.66
29	v	618	BCR	C15-C14-C13	-2.53	123.70	127.31
34	BF	518	DGD	O5D-C6D-C5D	-2.53	104.37	109.05
24	BQ	614	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	z	102	BCR	C15-C14-C13	-2.53	123.70	127.31
24	Y	305	CLA	C1-C2-C3	-2.53	122.66	126.75
23	BV	607	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
24	n	602	CLA	C3B-C4B-NB	-2.53	108.17	110.52
27	L	102	LHG	C11-C10-C9	-2.53	101.60	114.42
23	6	601	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
23	S	605	CHL	C2A-C1A-CHA	-2.53	119.44	123.86
24	5	602	CLA	CHB-C4A-NA	2.53	128.00	124.51
23	g	601	CHL	C2A-C1A-CHA	-2.53	119.44	123.86
24	BB	305	CLA	C1-C2-C3	-2.53	122.67	126.75
24	s	613	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	BG	402	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
29	A	411	BCR	C27-C26-C25	2.53	126.40	122.73
23	e	601	CHL	C2A-C1A-CHA	-2.52	119.44	123.86
28	G	619	XAT	C20-C13-C12	-2.52	114.10	118.08
23	9	609	CHL	O2D-CGD-O1D	-2.52	118.90	123.84
23	BQ	609	CHL	OMC-CMC-C2C	-2.52	119.98	125.69
24	BU	603	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
23	y	302	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
27	Az	102	LHG	C11-C10-C9	-2.52	101.62	114.42
29	1	515	BCR	C15-C14-C13	-2.52	123.71	127.31
23	9	607	CHL	C4-C3-C5	2.52	119.51	115.27
29	BD	411	BCR	C27-C26-C25	2.52	126.39	122.73
27	2	406	LHG	C11-C10-C9	-2.52	101.62	114.42
27	C	521	LHG	C20-C19-C18	-2.52	101.62	114.42
23	BJ	608	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
23	Y	306	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
24	AB	310	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
24	b	605	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	BJ	603	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	R	404	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
23	G	601	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
26	BV	616	NEX	C28-C29-C30	2.52	122.81	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	404	LHG	O8-C23-C24	2.52	119.81	111.91
27	1	520	LHG	O8-C23-C24	2.52	119.81	111.91
23	r	606	CHL	C3D-C4D-ND	2.52	114.31	110.24
23	0	601	CHL	CMD-C2D-C3D	-2.52	121.82	127.61
23	BU	607	CHL	C4-C3-C5	2.52	119.51	115.27
23	BB	308	CHL	C2A-C1A-CHA	-2.52	119.45	123.86
23	7	307	CHL	C1D-ND-C4D	-2.52	104.55	106.33
23	G	609	CHL	C4-C3-C5	2.52	119.51	115.27
23	Au	608	CHL	C4-C3-C5	2.52	119.51	115.27
24	c	510	CLA	C3B-C4B-NB	-2.52	108.18	110.52
24	g	614	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	n	607	CHL	C1-C2-C3	-2.52	121.69	126.04
24	BQ	612	CLA	CHB-C4A-NA	2.52	127.99	124.51
24	BD	410	CLA	CHB-C4A-NA	2.52	127.99	124.51
27	Ba	319	LHG	C11-C10-C9	-2.52	101.65	114.42
27	d	404	LHG	C11-C10-C9	-2.52	101.66	114.42
32	Az	101	SQD	O48-C23-C24	2.52	119.80	111.91
33	F	102	HEM	C1B-NB-C4B	2.52	107.67	105.07
25	AA	317	LUT	C35-C15-C14	2.52	128.63	123.47
27	BY	201	LHG	C11-C10-C9	-2.52	101.66	114.42
24	a	410	CLA	CHB-C4A-NA	2.51	127.99	124.51
30	BE	621	LMG	O1-C1-C2	-2.51	104.38	108.30
23	A2	605	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
24	v	608	CLA	CHB-C4A-NA	2.51	127.99	124.51
25	n	616	LUT	C12-C13-C14	2.51	122.80	118.94
23	0	606	CHL	CMD-C2D-C3D	-2.51	121.83	127.61
24	BJ	614	CLA	CHB-C4A-NA	2.51	127.99	124.51
25	y	317	LUT	C12-C13-C14	2.51	122.80	118.94
29	B	617	BCR	C11-C10-C9	-2.51	123.72	127.31
24	1	505	CLA	C3B-C4B-NB	-2.51	108.19	110.52
27	5	618	LHG	C20-C19-C18	-2.51	101.67	114.42
25	BV	615	LUT	C39-C29-C28	2.51	122.03	118.08
29	B	618	BCR	C15-C14-C13	-2.51	123.73	127.31
29	a	411	BCR	C27-C26-C25	2.51	126.38	122.73
25	r	615	LUT	C35-C15-C14	2.51	128.62	123.47
30	2	407	LMG	O1-C7-C8	-2.51	104.84	110.90
25	N	616	LUT	C32-C33-C34	2.51	122.79	118.94
24	6	604	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	8	310	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	BQ	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	r	606	CHL	C1-C2-C3	-2.51	121.70	126.04
24	Y	303	CLA	C3B-C4B-NB	-2.51	108.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BQ	608	CHL	OMC-CMC-C2C	-2.51	120.01	125.69
24	9	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	BD	405	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	BG	405	LMG	O1-C7-C8	-2.51	104.84	110.90
24	Y	311	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	0	604	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
31	2	404	PL9	C27-C28-C29	-2.51	121.62	127.66
23	A6	605	CHL	C2A-C1A-CHA	-2.51	119.47	123.86
24	BU	602	CLA	CAC-C3C-C4C	2.51	128.07	124.81
24	S	612	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	BB	304	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	9	618	LHG	C20-C19-C18	-2.51	101.69	114.42
24	A	405	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	BU	606	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
24	r	609	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	BV	611	CLA	C3B-C4B-NB	-2.51	108.19	110.52
27	BG	404	LHG	C11-C10-C9	-2.51	101.69	114.42
25	AA	317	LUT	C12-C13-C14	2.51	122.79	118.94
23	Au	601	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
25	Y	316	LUT	C12-C13-C14	2.51	122.79	118.94
24	S	609	CLA	CHB-C1B-NB	2.51	126.91	124.26
24	d	402	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
23	BJ	601	CHL	C2A-C1A-CHA	-2.51	119.48	123.86
24	1	503	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	A0	201	LMG	C40-C39-C38	-2.51	101.70	114.42
23	0	607	CHL	O2A-CGA-CBA	2.51	119.77	111.91
24	0	613	CLA	C3B-C4B-NB	-2.51	108.19	110.52
30	BL	101	LMG	C40-C39-C38	-2.51	101.70	114.42
34	c	517	DGD	O5D-C6D-C5D	-2.51	104.41	109.05
27	b	623	LHG	C11-C10-C9	-2.51	101.70	114.42
23	BQ	607	CHL	C1-C2-C3	-2.51	121.71	126.04
24	G	602	CLA	C3B-C4B-NB	-2.51	108.19	110.52
24	BB	311	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	BJ	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	1	520	LHG	C11-C10-C9	-2.50	101.71	114.42
24	9	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	n	608	CHL	OMC-CMC-C2C	-2.50	120.03	125.69
23	BV	605	CHL	O2D-CGD-O1D	-2.50	118.94	123.84
24	BJ	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
32	L	101	SQD	O48-C23-C24	2.50	119.76	111.91
24	BE	612	CLA	C3B-C4B-NB	-2.50	108.19	110.52
24	BJ	604	CLA	C3B-C4B-NB	-2.50	108.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	501	LMG	C40-C39-C38	-2.50	101.72	114.42
29	c	515	BCR	C33-C5-C6	-2.50	121.72	124.53
30	i	101	LMG	C40-C39-C38	-2.50	101.72	114.42
24	BE	616	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	S	612	CLA	C3B-C4B-NB	-2.50	108.19	110.52
24	BJ	602	CLA	C3B-C4B-NB	-2.50	108.19	110.52
27	d	404	LHG	O8-C23-C24	2.50	119.76	111.91
27	BF	520	LHG	O8-C23-C24	2.50	119.76	111.91
24	n	613	CLA	C3B-C4B-NB	-2.50	108.19	110.52
24	g	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	S	603	CLA	C3B-C4B-NB	-2.50	108.20	110.52
27	w	201	LHG	C11-C10-C9	-2.50	101.73	114.42
23	Au	609	CHL	O2A-CGA-CBA	2.50	119.75	111.91
29	BF	516	BCR	C7-C8-C9	-2.50	122.46	126.23
23	6	609	CHL	C3D-C4D-ND	2.50	114.28	110.24
24	BQ	613	CLA	C3B-C4B-NB	-2.50	108.20	110.52
29	c	515	BCR	C27-C26-C25	2.50	126.36	122.73
23	5	607	CHL	C4-C3-C5	2.50	119.47	115.27
24	g	604	CLA	C3B-C4B-NB	-2.50	108.20	110.52
24	6	611	CLA	O2D-CGD-CBD	2.50	115.70	111.27
24	B	608	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	9	606	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
23	r	605	CHL	C4A-NA-C1A	2.50	107.83	106.71
24	G	604	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	BB	309	CHL	C4-C3-C5	2.50	119.47	115.27
28	8	312	XAT	C25-C24-C23	-2.50	107.81	112.75
24	AB	302	CLA	C3B-C4B-NB	-2.50	108.20	110.52
30	A	412	LMG	C40-C39-C38	-2.50	101.76	114.42
28	9	619	XAT	C20-C13-C14	-2.50	119.43	122.92
24	AB	308	CLA	CHB-C1B-NB	2.49	126.90	124.26
24	A6	612	CLA	C3B-C4B-NB	-2.49	108.20	110.52
24	BB	314	CLA	C3B-C4B-NB	-2.49	108.20	110.52
27	C	520	LHG	O8-C23-C24	2.49	119.73	111.91
24	b	616	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	y	317	LUT	C32-C33-C34	2.49	122.77	118.94
24	9	602	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
23	Au	605	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
24	AA	313	CLA	CHB-C1B-NB	2.49	126.90	124.26
24	BE	615	CLA	O2D-CGD-CBD	2.49	115.70	111.27
24	1	506	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	A6	605	CHL	OMC-CMC-C2C	-2.49	120.05	125.69
23	g	605	CHL	C2A-C1A-CHA	-2.49	119.50	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	g	607	CHL	C2A-C1A-CHA	-2.49	119.50	123.86
23	0	605	CHL	CHC-C4B-NB	-2.49	121.62	124.26
25	5	616	LUT	C39-C29-C28	2.49	122.00	118.08
23	Y	310	CHL	C1D-ND-C4D	-2.49	104.56	106.33
23	Au	609	CHL	C4-C3-C5	2.49	119.46	115.27
23	9	605	CHL	C4A-NA-C1A	2.49	107.83	106.71
30	C	501	LMG	C40-C39-C38	-2.49	101.78	114.42
23	G	608	CHL	C4-C3-C5	2.49	119.46	115.27
23	S	606	CHL	C4-C3-C5	2.49	119.46	115.27
23	r	607	CHL	C4-C3-C5	2.49	119.46	115.27
29	BE	618	BCR	C37-C22-C21	-2.49	119.43	122.92
24	r	602	CLA	C3B-C4B-NB	-2.49	108.20	110.52
29	C	515	BCR	C33-C5-C6	-2.49	121.73	124.53
27	BU	617	LHG	C20-C19-C18	-2.49	101.78	114.42
23	Y	309	CHL	C4-C3-C5	2.49	119.46	115.27
27	BE	623	LHG	C11-C10-C9	-2.49	101.79	114.42
24	B	601	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	B	623	BCR	C24-C23-C22	-2.49	122.47	126.23
30	C	501	LMG	O6-C1-O1	-2.49	104.08	109.97
23	0	606	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
33	F	102	HEM	C4C-NC-C1C	2.49	107.78	105.35
23	S	605	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
23	BB	302	CHL	C2A-C1A-CHA	-2.49	119.51	123.86
24	AA	314	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	G	618	LHG	C11-C10-C9	-2.49	101.80	114.42
29	C	515	BCR	C15-C14-C13	-2.49	123.76	127.31
23	9	607	CHL	CMD-C2D-C3D	-2.49	121.89	127.61
23	6	608	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
30	1	519	LMG	C40-C39-C38	-2.49	101.80	114.42
24	R	406	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	G	609	CHL	O2A-CGA-CBA	2.49	119.71	111.91
24	v	609	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
38	BD	409	PHO	C1-C2-C3	-2.49	121.74	126.04
23	Ba	302	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
24	5	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	1	512	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	BQ	610	CLA	CHD-C1D-ND	-2.49	122.17	124.45
24	r	603	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
24	9	602	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	b	602	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	b	608	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	N	610	CLA	CMB-C2B-C1B	-2.48	121.59	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	r	606	CHL	C1C-C2C-C3C	-2.48	105.14	107.11
24	A6	611	CLA	C3B-C4B-NB	-2.48	108.21	110.52
24	BU	604	CLA	O2D-CGD-CBD	2.48	115.68	111.27
24	Au	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
31	d	403	PL9	C32-C31-C29	2.48	121.14	112.98
29	Bb	101	BCR	C38-C26-C25	-2.48	121.74	124.53
24	BU	609	CLA	CHC-C4B-NB	2.48	126.89	124.26
27	n	618	LHG	C20-C19-C18	-2.48	101.82	114.42
24	n	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
38	a	409	PHO	C1-C2-C3	-2.48	121.75	126.04
27	b	622	LHG	C11-C10-C9	-2.48	101.83	114.42
27	2	406	LHG	C20-C19-C18	-2.48	101.83	114.42
38	BD	409	PHO	CMB-C2B-C3B	2.48	129.32	124.68
29	b	620	BCR	C24-C23-C22	-2.48	122.49	126.23
29	Ay	101	BCR	C24-C23-C22	-2.48	122.49	126.23
30	1	501	LMG	O6-C1-O1	-2.48	104.10	109.97
29	Ay	101	BCR	C33-C5-C6	-2.48	121.74	124.53
27	C	520	LHG	C11-C10-C9	-2.48	101.84	114.42
23	AB	307	CHL	CHD-C1D-C2D	2.48	130.68	125.48
33	4	102	HEM	C4C-NC-C1C	2.48	107.78	105.35
24	A	407	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	g	618	LHG	C11-C10-C9	-2.48	101.84	114.42
24	A2	610	CLA	C1-C2-C3	-2.48	121.76	126.04
23	8	306	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
27	BJ	618	LHG	C20-C19-C18	-2.48	101.85	114.42
23	y	306	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
29	k	101	BCR	C24-C23-C22	-2.48	122.49	126.23
24	7	314	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	C	512	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	v	601	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	BE	622	LHG	C11-C10-C9	-2.48	101.85	114.42
29	z	102	BCR	C38-C26-C25	-2.48	121.75	124.53
27	BJ	618	LHG	C11-C10-C9	-2.48	101.85	114.42
24	BE	605	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	BB	303	CLA	C3B-C4B-NB	-2.48	108.22	110.52
24	r	609	CLA	CHC-C4B-NB	2.48	126.88	124.26
23	AB	306	CHL	CMD-C2D-C3D	-2.48	121.92	127.61
29	K	102	BCR	C15-C14-C13	-2.48	123.78	127.31
24	r	611	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
30	D	405	LMG	O1-C7-C8	-2.48	104.93	110.90
24	Au	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	BE	621	LMG	C40-C39-C38	-2.48	101.86	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BD	411	BCR	C33-C5-C6	-2.47	121.75	124.53
29	f	101	BCR	C27-C26-C25	2.47	126.32	122.73
23	s	606	CHL	C2A-C1A-CHA	-2.47	119.53	123.86
24	8	303	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	g	602	CLA	C3B-C4B-NB	-2.47	108.22	110.52
24	v	604	CLA	C3B-C4B-NB	-2.47	108.22	110.52
24	r	602	CLA	CAC-C3C-C4C	2.47	128.02	124.81
23	s	605	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
27	BQ	618	LHG	C20-C19-C18	-2.47	101.88	114.42
29	a	411	BCR	C33-C5-C6	-2.47	121.75	124.53
29	BF	516	BCR	C33-C5-C6	-2.47	121.75	124.53
27	BE	624	LHG	C20-C19-C18	-2.47	101.88	114.42
23	A2	608	CHL	CHC-C4B-NB	-2.47	121.64	124.26
27	c	519	LHG	O8-C23-C24	2.47	119.66	111.91
23	6	601	CHL	C6-C5-C3	-2.47	110.58	114.62
29	Ay	102	BCR	C38-C26-C25	-2.47	121.75	124.53
24	B	604	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	AB	302	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	n	607	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
24	8	302	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	B	605	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	G	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	r	618	LHG	C20-C19-C18	-2.47	101.89	114.42
24	BF	504	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	BU	601	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
23	BU	607	CHL	C1-C2-C3	-2.47	121.77	126.04
23	Ba	310	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
24	R	404	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
23	BQ	607	CHL	C1C-C2C-C3C	-2.47	105.16	107.11
23	Y	308	CHL	C2A-C1A-CHA	-2.47	119.55	123.86
24	A6	603	CLA	C3B-C4B-NB	-2.47	108.23	110.52
24	8	301	CLA	CMC-C2C-C1C	2.47	128.79	125.04
30	v	620	LMG	C38-C37-C36	-2.47	101.91	114.42
24	BE	609	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
23	BJ	605	CHL	C2A-C1A-CHA	-2.47	119.55	123.86
27	g	618	LHG	C20-C19-C18	-2.47	101.91	114.42
24	g	604	CLA	CHB-C4A-NA	2.47	127.92	124.51
27	BG	404	LHG	O8-C23-C24	2.46	119.64	111.91
27	Au	618	LHG	C11-C10-C9	-2.46	101.91	114.42
30	C	519	LMG	C40-C39-C38	-2.46	101.91	114.42
24	Ba	305	CLA	CHB-C4A-NA	2.46	127.92	124.51
29	BI	101	BCR	C27-C26-C25	2.46	126.31	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N	618	LHG	C11-C10-C9	-2.46	101.92	114.42
33	f	102	HEM	C4A-NA-C1A	2.46	107.76	105.35
25	G	616	LUT	C8-C9-C10	2.46	122.72	118.94
23	G	607	CHL	C6-C5-C3	-2.46	110.59	114.62
24	v	605	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	6	607	CHL	O2A-CGA-CBA	2.46	119.64	111.91
23	BV	606	CHL	C2A-C1A-CHA	-2.46	119.55	123.86
24	y	311	CLA	O2D-CGD-CBD	2.46	115.64	111.27
29	BN	101	BCR	C24-C23-C22	-2.46	122.51	126.23
24	Au	613	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	6	615	LUT	C39-C29-C28	2.46	121.96	118.08
27	D	404	LHG	C20-C19-C18	-2.46	101.93	114.42
23	7	310	CHL	O1D-CGD-CBD	-2.46	119.45	124.48
28	Au	619	XAT	C20-C13-C12	-2.46	114.20	118.08
24	AA	313	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	A6	606	CHL	O1D-CGD-CBD	-2.46	119.45	124.48
23	BU	606	CHL	C1-C2-C3	-2.46	121.79	126.04
29	4	101	BCR	C27-C26-C25	2.46	126.30	122.73
24	c	504	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	v	603	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	b	621	LMG	C40-C39-C38	-2.46	101.94	114.42
24	BG	401	CLA	O2D-CGD-CBD	2.46	115.64	111.27
23	BQ	609	CHL	CBC-CAC-C3C	-2.46	105.66	112.43
24	C	503	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	Y	308	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
24	b	615	CLA	O2D-CGD-CBD	2.46	115.63	111.27
23	N	608	CHL	CHC-C4B-NB	-2.46	121.66	124.26
23	A6	606	CHL	C4-C3-C5	2.46	119.40	115.27
30	b	621	LMG	O1-C1-C2	-2.46	104.47	108.30
32	A	413	SQD	O48-C23-C24	2.46	119.61	111.91
23	y	302	CHL	CHC-C4B-NB	-2.46	121.66	124.26
25	S	615	LUT	C31-C30-C29	2.46	130.81	127.31
24	BE	602	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	AB	308	CLA	CHD-C1D-ND	-2.45	122.20	124.45
23	S	601	CHL	O2D-CGD-O1D	-2.45	119.04	123.84
23	5	609	CHL	O1D-CGD-CBD	-2.45	119.46	124.48
24	S	608	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
23	BB	308	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
24	A6	604	CLA	C1-C2-C3	-2.45	122.78	126.75
24	Au	610	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
24	A	405	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
30	B	620	LMG	C38-C37-C36	-2.45	101.98	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BD	411	BCR	C24-C23-C22	-2.45	122.53	126.23
24	BU	601	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
24	n	614	CLA	O2D-CGD-CBD	2.45	115.62	111.27
24	v	616	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
27	B	621	LHG	C11-C10-C9	-2.45	101.98	114.42
23	BU	613	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
24	v	612	CLA	CHC-C4B-NB	2.45	126.85	124.26
24	A6	608	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
23	0	609	CHL	C4-C3-C5	2.45	119.39	115.27
27	1	520	LHG	C20-C19-C18	-2.45	101.99	114.42
24	0	613	CLA	C2D-C1D-ND	-2.45	108.30	110.10
23	7	302	CHL	C3B-C4B-NB	2.45	112.79	110.52
25	BV	615	LUT	C32-C33-C34	2.45	122.70	118.94
25	BU	615	LUT	C8-C9-C10	2.45	122.70	118.94
32	R	411	SQD	O48-C23-C24	2.45	119.59	111.91
24	Ba	311	CLA	O2D-CGD-CBD	2.45	115.62	111.27
23	r	607	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
31	BG	403	PL9	O1-C4-C3	-2.45	118.02	120.72
24	S	608	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A6	606	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
30	d	405	LMG	O1-C7-C8	-2.45	104.99	110.90
30	v	623	LMG	O6-C1-O1	-2.45	104.18	109.97
25	A6	615	LUT	C31-C30-C29	2.45	130.80	127.31
24	A6	608	CLA	CHB-C4A-NA	2.45	127.89	124.51
24	6	604	CLA	CHB-C4A-NA	2.45	127.89	124.51
24	7	305	CLA	CHB-C1B-NB	2.45	126.85	124.26
23	S	606	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
27	B	622	LHG	C11-C10-C9	-2.45	102.01	114.42
30	BF	519	LMG	C40-C39-C38	-2.44	102.01	114.42
23	BJ	606	CHL	C1C-C2C-C3C	-2.44	105.17	107.11
24	0	611	CLA	O2D-CGD-CBD	2.44	115.61	111.27
24	g	610	CLA	C1-C2-C3	-2.44	121.82	126.04
30	c	518	LMG	C40-C39-C38	-2.44	102.02	114.42
24	6	610	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	A6	615	LUT	C35-C15-C14	2.44	128.48	123.47
23	AA	307	CHL	C1D-ND-C4D	-2.44	104.60	106.33
23	BU	606	CHL	OMC-CMC-C2C	-2.44	120.16	125.69
27	A2	618	LHG	C11-C10-C9	-2.44	102.02	114.42
27	BF	521	LHG	C20-C19-C18	-2.44	102.02	114.42
24	5	612	CLA	CHB-C1B-NB	2.44	126.84	124.26
23	BU	606	CHL	C3D-C4D-ND	2.44	114.19	110.24
29	c	515	BCR	C11-C10-C9	-2.44	123.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	402	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	AB	307	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
23	BV	606	CHL	CMD-C2D-C3D	-2.44	122.00	127.61
24	r	612	CLA	C3B-C4B-NB	-2.44	108.25	110.52
23	Au	601	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
23	Au	608	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
23	BB	302	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
25	n	615	LUT	C12-C13-C14	2.44	122.68	118.94
23	6	605	CHL	CHC-C4B-NB	-2.44	121.67	124.26
24	BQ	614	CLA	O2D-CGD-CBD	2.44	115.60	111.27
25	Ba	317	LUT	C32-C33-C34	2.44	122.68	118.94
24	c	505	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	BD	410	CLA	C3B-C4B-NB	-2.44	108.25	110.52
27	BF	520	LHG	C11-C10-C9	-2.44	102.06	114.42
23	y	310	CHL	O2A-CGA-CBA	2.44	119.55	111.91
28	5	619	XAT	C5-C4-C3	-2.44	107.93	112.75
23	BQ	609	CHL	C1D-ND-C4D	-2.44	104.61	106.33
24	9	612	CLA	CHB-C1B-NB	2.44	126.83	124.26
23	s	601	CHL	CMD-C2D-C3D	-2.43	122.01	127.61
23	Ba	306	CHL	C1C-C2C-C3C	-2.43	105.18	107.11
27	c	520	LHG	C20-C19-C18	-2.43	102.07	114.42
23	g	601	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
23	BV	601	CHL	CMD-C2D-C3D	-2.43	122.02	127.61
27	v	621	LHG	C11-C10-C9	-2.43	102.07	114.42
24	AA	305	CLA	CHB-C1B-NB	2.43	126.83	124.26
24	n	604	CLA	C1-C2-C3	-2.43	122.81	126.75
24	R	409	CLA	C3B-C4B-NB	-2.43	108.26	110.52
25	5	616	LUT	C12-C13-C14	2.43	122.67	118.94
24	N	613	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	y	305	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	AB	308	CLA	C2A-C3A-C4A	2.43	105.80	101.87
24	AB	301	CLA	CMC-C2C-C1C	2.43	128.74	125.04
34	Av	102	DGD	C1D-C2D-C3D	-2.43	104.93	110.00
23	Au	607	CHL	C6-C5-C3	-2.43	110.64	114.62
24	5	610	CLA	CHB-C1B-NB	2.43	126.83	124.26
27	2	406	LHG	O8-C23-C24	2.43	119.54	111.91
27	C	520	LHG	C20-C19-C18	-2.43	102.08	114.42
24	BE	609	CLA	CAA-CBA-CGA	-2.43	106.15	113.25
24	BU	610	CLA	C3B-C4B-NB	-2.43	108.26	110.52
24	n	613	CLA	C1-C2-C3	-2.43	121.84	126.04
23	S	607	CHL	C4A-NA-C1A	2.43	107.80	106.71
25	AA	317	LUT	C32-C33-C34	2.43	122.67	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	314	CLA	C3B-C4B-NB	-2.43	108.26	110.52
23	S	606	CHL	O1D-CGD-CBD	-2.43	119.52	124.48
23	S	606	CHL	C1C-C2C-C3C	-2.43	105.19	107.11
27	b	624	LHG	C20-C19-C18	-2.43	102.10	114.42
24	B	616	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
24	B	608	CLA	CHB-C1B-NB	2.43	126.83	124.26
24	0	612	CLA	C3B-C4B-NB	-2.43	108.26	110.52
23	BJ	609	CHL	CHD-C4C-C3C	-2.43	121.27	124.84
24	C	512	CLA	C1-C2-C3	-2.43	121.85	126.04
27	2	405	LHG	C11-C10-C9	-2.43	102.11	114.42
29	F	101	BCR	C27-C26-C25	2.43	126.25	122.73
23	BB	306	CHL	C4D-CHA-C1A	-2.43	118.30	121.25
24	v	604	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	9	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
23	BB	309	CHL	CAA-C2A-C3A	-2.43	106.14	112.78
24	Ba	312	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	r	610	CLA	C3B-C4B-NB	-2.43	108.27	110.52
29	BF	516	BCR	C11-C10-C9	-2.43	123.85	127.31
24	y	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	r	606	CHL	OMC-CMC-C2C	-2.42	120.20	125.69
29	4	101	BCR	C24-C23-C22	-2.42	122.57	126.23
24	BG	401	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
24	c	510	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	BJ	610	CLA	C1-C2-C3	-2.42	121.85	126.04
29	C	515	BCR	C11-C10-C9	-2.42	123.85	127.31
23	n	606	CHL	C4A-NA-C1A	2.42	107.80	106.71
23	AA	310	CHL	O1D-CGD-CBD	-2.42	119.53	124.48
30	B	624	LMG	O6-C1-O1	-2.42	104.24	109.97
38	A	408	PHO	C1-C2-C3	-2.42	121.86	126.04
29	B	618	BCR	C33-C5-C6	-2.42	121.81	124.53
23	9	609	CHL	C3D-C4D-ND	2.42	114.15	110.24
24	B	611	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	S	615	LUT	C35-C15-C14	2.42	128.43	123.47
23	g	606	CHL	C1C-C2C-C3C	-2.42	105.19	107.11
23	Ba	310	CHL	O2A-CGA-CBA	2.42	119.50	111.91
24	BE	605	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
24	8	303	CLA	C3B-C4B-NB	-2.42	108.27	110.52
23	0	606	CHL	O1D-CGD-CBD	-2.42	119.53	124.48
25	s	615	LUT	C32-C33-C34	2.42	122.65	118.94
27	c	519	LHG	C11-C10-C9	-2.42	102.15	114.42
24	G	610	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	g	613	CLA	CHB-C4A-NA	2.42	127.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	614	LUT	C12-C13-C14	2.42	122.65	118.94
26	Y	318	NEX	C28-C29-C30	2.42	122.65	118.94
30	BE	621	LMG	C38-C37-C36	-2.42	102.16	114.42
29	f	101	BCR	C24-C23-C22	-2.42	122.58	126.23
23	AA	310	CHL	CHD-C4C-C3C	-2.42	121.29	124.84
24	A2	613	CLA	CHB-C4A-NA	2.42	127.85	124.51
24	BQ	604	CLA	C1-C2-C3	-2.42	122.84	126.75
29	v	618	BCR	C33-C5-C6	-2.42	121.82	124.53
34	a	401	DGD	C3G-C2G-C1G	-2.42	106.08	111.79
24	5	602	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
24	BU	612	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	7	310	CHL	CHD-C4C-C3C	-2.41	121.29	124.84
24	6	613	CLA	C3B-C4B-NB	-2.41	108.28	110.52
23	n	609	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
24	R	405	CLA	C1-C2-C3	-2.41	121.87	126.04
24	0	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	a	410	CLA	C3B-C4B-NB	-2.41	108.28	110.52
24	AB	303	CLA	C3B-C4B-NB	-2.41	108.28	110.52
31	d	403	PL9	C35-C34-C36	2.41	119.33	115.27
23	A6	601	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
24	BJ	613	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	n	608	CHL	C4A-NA-C1A	2.41	107.79	106.71
24	g	612	CLA	CHB-C4A-NA	2.41	127.85	124.51
29	K	101	BCR	C24-C23-C22	-2.41	122.59	126.23
33	f	102	HEM	C1B-NB-C4B	2.41	107.56	105.07
23	9	609	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
23	g	609	CHL	CHD-C4C-C3C	-2.41	121.30	124.84
24	Y	312	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	r	602	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	0	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	1	512	CLA	C1-C2-C3	-2.41	121.88	126.04
29	K	102	BCR	C38-C26-C25	-2.41	121.82	124.53
24	BF	512	CLA	C1-C2-C3	-2.41	121.88	126.04
24	b	615	CLA	C3B-C4B-NB	-2.41	108.28	110.52
24	A	410	CLA	C3B-C4B-NB	-2.41	108.28	110.52
30	b	621	LMG	C38-C37-C36	-2.41	102.20	114.42
23	G	606	CHL	CAA-C2A-C1A	2.41	119.86	111.97
23	5	608	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
25	Y	317	LUT	C32-C33-C34	2.41	122.63	118.94
34	H	102	DGD	C1D-C2D-C3D	-2.41	104.98	110.00
30	Aw	101	LMG	C38-C37-C36	-2.41	102.21	114.42
24	5	603	CLA	CHB-C1B-NB	2.40	126.80	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	r	605	CHL	C3C-C4C-NC	2.40	113.27	110.57
27	A0	202	LHG	C11-C10-C9	-2.40	102.22	114.42
24	BF	510	CLA	CHB-C4A-NA	2.40	127.84	124.51
23	A6	606	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
24	5	610	CLA	CAC-C3C-C4C	2.40	127.93	124.81
23	G	601	CHL	C2A-C1A-CHA	-2.40	119.66	123.86
24	AB	310	CLA	C3B-C4B-NB	-2.40	108.29	110.52
24	AB	301	CLA	CHD-C1D-ND	-2.40	122.25	124.45
27	N	618	LHG	C20-C19-C18	-2.40	102.23	114.42
27	W	201	LHG	C11-C10-C9	-2.40	102.23	114.42
38	R	407	PHO	C1-C2-C3	-2.40	121.89	126.04
30	I	101	LMG	C38-C37-C36	-2.40	102.23	114.42
30	B	620	LMG	C40-C39-C38	-2.40	102.23	114.42
29	BI	101	BCR	C24-C23-C22	-2.40	122.61	126.23
23	Ba	309	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
23	s	606	CHL	CMD-C2D-C3D	-2.40	122.09	127.61
27	BF	520	LHG	C20-C19-C18	-2.40	102.23	114.42
23	s	605	CHL	C4D-CHA-C1A	-2.40	118.33	121.25
24	BF	505	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	y	309	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
23	y	310	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
24	s	609	CLA	C3B-C4B-NB	-2.40	108.29	110.52
27	c	520	LHG	C11-C10-C9	-2.40	102.24	114.42
25	BV	614	LUT	C12-C13-C14	2.40	122.62	118.94
25	Ba	316	LUT	C12-C13-C14	2.40	122.62	118.94
25	5	616	LUT	C31-C30-C29	2.40	130.74	127.31
27	BF	521	LHG	C11-C10-C9	-2.40	102.24	114.42
24	b	609	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	9	619	XAT	C5-C4-C3	-2.40	108.00	112.75
24	BB	312	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	9	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
33	BI	102	HEM	C4A-NA-C1A	2.40	107.70	105.35
23	N	607	CHL	C2A-C1A-CHA	-2.40	119.67	123.86
23	r	606	CHL	C6-C5-C3	-2.40	110.70	114.62
30	v	620	LMG	C40-C39-C38	-2.40	102.26	114.42
23	Au	606	CHL	CAA-C2A-C1A	2.40	119.83	111.97
30	v	620	LMG	O1-C7-C8	-2.40	105.12	110.90
23	Ba	302	CHL	CHC-C4B-NB	-2.40	121.72	124.26
24	AA	312	CLA	CHB-C1B-NB	2.40	126.79	124.26
23	BJ	601	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
23	BJ	608	CHL	C2A-C1A-CHA	-2.40	119.67	123.86
23	g	608	CHL	C1C-C2C-C3C	-2.40	105.21	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	BI	102	HEM	C1B-NB-C4B	2.40	107.55	105.07
24	AB	303	CLA	CHB-C4A-NA	2.40	127.82	124.51
24	v	608	CLA	CHB-C1B-NB	2.39	126.79	124.26
30	BF	501	LMG	C40-C39-C38	-2.39	102.27	114.42
27	1	521	LHG	C11-C10-C9	-2.39	102.27	114.42
29	v	622	BCR	C24-C23-C22	-2.39	122.62	126.23
34	h	102	DGD	C3G-C2G-C1G	-2.39	106.13	111.79
24	v	604	CLA	C1-C2-C3	-2.39	121.90	126.04
24	c	505	CLA	CHD-C1D-ND	-2.39	122.25	124.45
23	r	607	CHL	C1-C2-C3	-2.39	121.91	126.04
32	Az	101	SQD	O5-C1-O6	-2.39	104.31	109.97
24	b	605	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
30	c	501	LMG	C40-C39-C38	-2.39	102.28	114.42
23	A2	607	CHL	C2A-C1A-CHA	-2.39	119.68	123.86
23	g	608	CHL	C2A-C1A-CHA	-2.39	119.68	123.86
29	a	411	BCR	C24-C23-C22	-2.39	122.62	126.23
38	R	408	PHO	C1-C2-C3	-2.39	121.91	126.04
27	2	406	LHG	C18-C17-C16	-2.39	102.29	114.42
24	5	603	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	B	604	CLA	C3B-C4B-NB	-2.39	108.30	110.52
23	6	609	CHL	C4-C3-C5	2.39	119.29	115.27
23	9	606	CHL	CHB-C4A-NA	2.39	127.82	124.51
25	y	316	LUT	C32-C33-C34	2.39	122.61	118.94
25	BQ	615	LUT	C12-C13-C14	2.39	122.61	118.94
23	Y	306	CHL	C4D-CHA-C1A	-2.39	118.34	121.25
24	6	613	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	S	601	CHL	CMD-C2D-C3D	-2.39	122.12	127.61
27	A2	618	LHG	C20-C19-C18	-2.39	102.30	114.42
24	B	604	CLA	C1-C2-C3	-2.39	121.91	126.04
25	BJ	615	LUT	C32-C33-C34	2.39	122.60	118.94
25	7	317	LUT	C39-C29-C28	2.39	121.84	118.08
27	c	519	LHG	C20-C19-C18	-2.39	102.31	114.42
25	6	616	LUT	C28-C29-C30	2.39	122.60	118.94
29	K	101	BCR	C27-C26-C25	2.39	126.19	122.73
28	BU	616	XAT	C5-C4-C3	-2.39	108.03	112.75
23	0	609	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
23	r	613	CHL	C2A-C1A-CHA	-2.39	119.69	123.85
24	B	612	CLA	CHC-C4B-NB	2.39	126.78	124.26
24	y	312	CLA	C1-C2-C3	-2.39	121.92	126.04
24	1	509	CLA	C1-C2-C3	-2.39	121.92	126.04
24	BE	606	CLA	CHB-C4A-NA	2.38	127.81	124.51
38	a	408	PHO	C1-C2-C3	-2.38	121.92	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	504	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	Y	307	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
25	N	615	LUT	C39-C29-C28	2.38	121.83	118.08
33	f	102	HEM	C4C-NC-C1C	2.38	107.68	105.35
23	Ba	308	CHL	C6-C5-C3	-2.38	110.72	114.62
30	B	620	LMG	O1-C7-C8	-2.38	105.15	110.90
23	8	307	CHL	C2A-C1A-CHA	-2.38	119.70	123.86
27	C	521	LHG	C11-C10-C9	-2.38	102.34	114.42
24	BQ	613	CLA	C1-C2-C3	-2.38	121.93	126.04
24	6	612	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	BV	605	CHL	C4D-CHA-C1A	-2.38	118.35	121.25
23	0	605	CHL	C1D-ND-C4D	-2.38	104.64	106.33
23	G	608	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
29	R	410	BCR	C15-C14-C13	-2.38	123.92	127.31
29	K	101	BCR	C8-C7-C6	-2.38	120.52	127.20
24	a	405	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
25	Ba	316	LUT	C32-C33-C34	2.38	122.59	118.94
24	6	610	CLA	CHD-C1D-ND	-2.38	122.27	124.45
24	r	611	CLA	CHB-C1B-NB	2.38	126.77	124.26
23	y	308	CHL	C6-C5-C3	-2.38	110.73	114.62
24	BB	314	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	BF	501	LMG	O6-C1-O1	-2.38	104.34	109.97
25	0	616	LUT	C28-C29-C30	2.38	122.59	118.94
24	a	406	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	A6	601	CHL	CMD-C2D-C3D	-2.38	122.15	127.61
24	9	610	CLA	CHD-C1D-ND	-2.38	122.27	124.45
23	6	605	CHL	C1D-ND-C4D	-2.37	104.65	106.33
26	BB	318	NEX	C28-C29-C30	2.37	122.58	118.94
34	R	401	DGD	O5D-C6D-C5D	-2.37	104.65	109.05
30	c	501	LMG	O6-C1-O1	-2.37	104.35	109.97
34	BD	401	DGD	C3G-C2G-C1G	-2.37	106.17	111.79
23	BU	607	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
23	AA	302	CHL	C3B-C4B-NB	2.37	112.72	110.52
23	6	601	CHL	C1D-ND-C4D	-2.37	104.65	106.33
27	G	618	LHG	C20-C19-C18	-2.37	102.40	114.42
23	9	605	CHL	C1D-ND-C4D	-2.37	104.65	106.33
24	r	601	CLA	CHB-C1B-NB	2.37	126.77	124.26
24	B	603	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	C	504	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	y	310	CHL	CHD-C1D-C2D	2.37	130.45	125.48
23	AA	310	CHL	C2D-C1D-ND	2.37	111.85	110.10
25	BB	317	LUT	C32-C33-C34	2.37	122.57	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	311	CLA	C1-C2-C3	-2.37	122.92	126.75
24	1	503	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
29	AB	313	BCR	C27-C26-C25	2.37	126.17	122.73
24	d	401	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
24	BJ	612	CLA	CHB-C1B-NB	2.37	126.76	124.26
24	N	613	CLA	CAC-C3C-C4C	2.37	127.88	124.81
23	n	601	CHL	CHC-C4B-NB	-2.37	121.75	124.26
24	B	612	CLA	C1-C2-C3	-2.36	121.95	126.04
23	r	613	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
23	G	607	CHL	C2A-C1A-CHA	-2.36	119.72	123.86
25	G	616	LUT	C32-C33-C34	2.36	122.57	118.94
25	n	616	LUT	C32-C33-C34	2.36	122.57	118.94
25	n	615	LUT	C39-C29-C28	2.36	121.80	118.08
23	8	307	CHL	CHC-C4B-NB	-2.36	121.76	124.26
24	r	612	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	2	402	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	BU	611	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	BU	612	CLA	C3B-C4B-NB	-2.36	108.33	110.52
23	A2	608	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
24	v	606	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
23	9	608	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
27	D	404	LHG	C18-C17-C16	-2.36	102.44	114.42
24	AA	305	CLA	CHB-C4A-NA	2.36	127.78	124.51
34	1	517	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	8	304	CHL	CHC-C4B-NB	-2.36	121.76	124.26
24	BU	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
23	BQ	607	CHL	CHB-C4A-NA	2.36	127.77	124.51
24	5	603	CLA	CHD-C1D-ND	-2.36	122.29	124.45
24	b	609	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
23	BJ	608	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
24	BQ	602	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	BE	615	CLA	C3B-C4B-NB	-2.36	108.33	110.52
24	9	604	CLA	CHB-C1B-C2B	-2.36	120.58	127.24
24	y	314	CLA	CHB-C4A-NA	2.36	127.77	124.51
30	i	101	LMG	C38-C37-C36	-2.36	102.47	114.42
29	v	622	BCR	C27-C26-C25	2.36	126.15	122.73
29	Ay	101	BCR	C7-C8-C9	-2.36	122.68	126.23
23	6	607	CHL	C1C-C2C-C3C	-2.36	105.25	107.11
23	Ba	308	CHL	C2A-C1A-CHA	-2.36	119.74	123.86
24	a	405	CLA	CHB-C4A-NA	2.35	127.77	124.51
34	A	402	DGD	O5D-C6D-C5D	-2.35	104.69	109.05
29	1	515	BCR	C11-C10-C9	-2.35	123.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	604	CLA	C3B-C4B-NB	-2.35	108.33	110.52
29	H	101	BCR	C7-C8-C9	-2.35	122.68	126.23
24	Y	314	CLA	CHB-C4A-NA	2.35	127.77	124.51
24	BJ	612	CLA	CHB-C4A-NA	2.35	127.77	124.51
30	c	518	LMG	C38-C37-C36	-2.35	102.48	114.42
24	BQ	611	CLA	C1-C2-C3	-2.35	121.97	126.04
23	9	607	CHL	O1D-CGD-CBD	-2.35	119.67	124.48
27	Y	319	LHG	C11-C10-C9	-2.35	102.48	114.42
24	b	606	CLA	CHB-C4A-NA	2.35	127.77	124.51
23	AA	309	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
25	g	615	LUT	C32-C33-C34	2.35	122.55	118.94
23	Ba	302	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
23	AB	304	CHL	CHC-C4B-NB	-2.35	121.77	124.26
24	g	612	CLA	CHB-C1B-NB	2.35	126.75	124.26
24	n	602	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	s	612	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	5	609	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
23	BB	307	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
29	a	411	BCR	C15-C16-C17	-2.35	118.66	123.47
24	A	406	CLA	C1-C2-C3	-2.35	121.98	126.04
29	b	619	BCR	C33-C5-C6	-2.35	121.89	124.53
23	s	605	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
23	G	609	CHL	C2D-C1D-ND	2.35	111.83	110.10
25	AA	316	LUT	C12-C13-C14	2.35	122.55	118.94
24	8	301	CLA	CHD-C1D-ND	-2.35	122.30	124.45
23	y	302	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
24	BV	612	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	s	607	CHL	C1D-ND-C4D	-2.35	104.67	106.33
30	2	407	LMG	O3-C3-C2	-2.35	104.92	110.35
30	BL	101	LMG	C38-C37-C36	-2.35	102.51	114.42
24	5	604	CLA	CHB-C1B-C2B	-2.35	120.61	127.24
25	Ba	317	LUT	C39-C29-C28	2.35	121.78	118.08
27	d	404	LHG	C20-C19-C18	-2.35	102.51	114.42
25	A6	614	LUT	C32-C33-C34	2.35	122.54	118.94
24	BU	614	CLA	C3B-C4B-NB	-2.35	108.34	110.52
23	5	605	CHL	C4A-NA-C1A	2.35	107.76	106.71
23	Y	302	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
30	BF	519	LMG	C38-C37-C36	-2.35	102.51	114.42
29	B	623	BCR	C27-C26-C25	2.35	126.14	122.73
24	C	511	CLA	CGD-CBD-CAD	2.35	118.33	110.73
27	1	521	LHG	C18-C17-C16	-2.35	102.51	114.42
27	Au	618	LHG	C20-C19-C18	-2.35	102.52	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BQ	601	CHL	CHC-C4B-NB	-2.35	121.77	124.26
24	AA	314	CLA	C3B-C4B-NB	-2.34	108.34	110.52
23	y	308	CHL	C2A-C1A-CHA	-2.34	119.76	123.86
24	BQ	613	CLA	CHB-C4A-NA	2.34	127.75	124.51
34	C	517	DGD	C3G-C2G-C1G	-2.34	106.25	111.79
24	BU	611	CLA	CHB-C1B-NB	2.34	126.74	124.26
23	g	608	CHL	C4-C3-C5	2.34	119.21	115.27
23	BJ	608	CHL	C4-C3-C5	2.34	119.21	115.27
27	BG	404	LHG	C18-C17-C16	-2.34	102.53	114.42
23	Au	607	CHL	C2A-C1A-CHA	-2.34	119.76	123.86
23	BU	613	CHL	C2A-C1A-CHA	-2.34	119.77	123.85
24	B	612	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
24	v	606	CLA	CHB-C1B-NB	2.34	126.73	124.26
27	Az	102	LHG	C20-C19-C18	-2.34	102.54	114.42
27	r	618	LHG	O8-C23-C24	2.34	119.25	111.91
34	BK	102	DGD	CBB-CAB-C9B	-2.34	102.55	114.42
23	AA	310	CHL	CHD-C1D-C2D	2.34	130.39	125.48
25	y	317	LUT	C39-C29-C28	2.34	121.76	118.08
27	L	102	LHG	C20-C19-C18	-2.34	102.55	114.42
23	AA	307	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
38	BD	408	PHO	C1-C2-C3	-2.34	122.00	126.04
30	D	405	LMG	O3-C3-C2	-2.34	104.94	110.35
24	8	308	CLA	CHD-C1D-ND	-2.34	122.31	124.45
24	n	613	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	2	407	LMG	O2-C2-C1	-2.34	104.37	110.05
23	BV	605	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
25	Au	616	LUT	C32-C33-C34	2.34	122.53	118.94
23	s	601	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
24	BQ	612	CLA	C3B-C4B-NB	-2.34	108.35	110.52
24	g	613	CLA	C1-C2-C3	-2.34	122.00	126.04
24	7	305	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	S	614	LUT	C32-C33-C34	2.33	122.52	118.94
24	BD	405	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
23	BV	607	CHL	C1D-ND-C4D	-2.33	104.68	106.33
34	c	517	DGD	C3G-C2G-C1G	-2.33	106.27	111.79
30	c	501	LMG	O3-C3-C2	-2.33	104.95	110.35
24	BU	614	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	BV	601	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
29	b	618	BCR	C38-C26-C27	-2.33	109.14	113.62
23	G	608	CHL	C1C-C2C-C3C	-2.33	105.26	107.11
24	v	612	CLA	C1-C2-C3	-2.33	122.01	126.04
24	Aw	102	CLA	CHB-C1B-NB	2.33	126.73	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Ay	101	BCR	C27-C26-C25	2.33	126.12	122.73
27	BG	404	LHG	C20-C19-C18	-2.33	102.59	114.42
23	7	310	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
23	7	310	CHL	CHD-C1D-C2D	2.33	130.37	125.48
23	Y	309	CHL	CAA-C2A-C3A	-2.33	106.39	112.78
23	0	601	CHL	C1D-ND-C4D	-2.33	104.68	106.33
27	Au	618	LHG	C27-C26-C25	-2.33	102.59	114.42
24	n	610	CLA	C3B-C4B-NB	-2.33	108.35	110.52
24	Ba	311	CLA	CHB-C4A-NA	2.33	127.73	124.51
29	Bb	101	BCR	C11-C10-C9	-2.33	123.98	127.31
23	n	609	CHL	CBC-CAC-C3C	-2.33	106.01	112.43
30	BF	501	LMG	O3-C3-C2	-2.33	104.97	110.35
30	C	501	LMG	C38-C37-C36	-2.33	102.61	114.42
25	A6	614	LUT	C12-C13-C14	2.33	122.51	118.94
30	D	405	LMG	O2-C2-C1	-2.33	104.39	110.05
24	5	610	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
27	C	521	LHG	C18-C17-C16	-2.33	102.61	114.42
29	A	411	BCR	C15-C14-C13	-2.33	123.99	127.31
23	G	605	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
23	N	608	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
24	BE	607	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
30	I	101	LMG	O3-C3-C2	-2.32	104.97	110.35
24	BD	405	CLA	C1-C2-C3	-2.32	122.02	126.04
24	C	503	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
23	Au	601	CHL	OMC-CMC-C2C	-2.32	120.43	125.69
23	BQ	608	CHL	C1D-ND-C4D	-2.32	104.68	106.33
23	8	306	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
23	n	607	CHL	CHB-C4A-NA	2.32	127.72	124.51
25	BV	615	LUT	C12-C13-C14	2.32	122.50	118.94
24	v	612	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
24	A2	610	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
27	d	404	LHG	C18-C17-C16	-2.32	102.65	114.42
25	AB	311	LUT	C35-C15-C14	2.32	128.22	123.47
27	BU	617	LHG	O8-C23-C24	2.32	119.18	111.91
23	7	309	CHL	C1C-C2C-C3C	-2.32	105.28	107.11
23	Au	609	CHL	C2A-C1A-CHA	-2.32	119.81	123.86
23	n	608	CHL	C1D-ND-C4D	-2.32	104.69	106.33
24	b	607	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
23	5	605	CHL	C1D-ND-C4D	-2.32	104.69	106.33
24	Ba	314	CLA	CHB-C4A-NA	2.32	127.71	124.51
24	7	312	CLA	CHB-C1B-NB	2.32	126.71	124.26
29	h	101	BCR	C3-C4-C5	-2.32	109.94	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	501	LMG	C38-C37-C36	-2.32	102.67	114.42
25	g	616	LUT	C8-C9-C10	2.31	122.49	118.94
24	7	314	CLA	C3B-C4B-NB	-2.31	108.37	110.52
24	y	311	CLA	CHB-C4A-NA	2.31	127.71	124.51
27	BU	617	LHG	C5-O7-C7	-2.31	112.10	117.79
27	y	319	LHG	C20-C19-C18	-2.31	102.68	114.42
23	8	304	CHL	C4D-CHA-C1A	-2.31	118.43	121.25
31	d	403	PL9	O1-C4-C3	-2.31	118.17	120.72
30	I	101	LMG	O6-C1-O1	-2.31	104.50	109.97
29	K	102	BCR	C11-C10-C9	-2.31	124.01	127.31
24	D	401	CLA	O2D-CGD-CBD	2.31	115.37	111.27
24	BD	406	CLA	C3B-C4B-NB	-2.31	108.37	110.52
24	A2	613	CLA	CAC-C3C-C4C	2.31	127.81	124.81
30	B	624	LMG	C38-C37-C36	-2.31	102.70	114.42
23	9	601	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
23	BV	605	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
29	z	102	BCR	C11-C10-C9	-2.31	124.02	127.31
29	BE	601	BCR	C27-C26-C25	2.31	126.08	122.73
24	BE	605	CLA	C3B-C4B-NB	-2.31	108.37	110.52
23	5	607	CHL	CHB-C4A-NA	2.31	127.70	124.51
24	A2	610	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
27	c	520	LHG	C18-C17-C16	-2.31	102.71	114.42
27	A2	618	LHG	C27-C26-C25	-2.31	102.71	114.42
30	v	623	LMG	C38-C37-C36	-2.31	102.71	114.42
24	5	602	CLA	CHB-C1B-NB	2.31	126.70	124.26
24	N	614	CLA	CHB-C1B-NB	2.31	126.70	124.26
29	BE	619	BCR	C33-C5-C6	-2.31	121.94	124.53
24	N	613	CLA	C1-C2-C3	-2.31	122.05	126.04
27	G	618	LHG	C27-C26-C25	-2.31	102.72	114.42
23	5	601	CHL	C2A-C1A-CHA	-2.31	119.83	123.86
32	L	101	SQD	O6-C44-C45	-2.31	105.33	110.90
25	5	615	LUT	C32-C33-C34	2.30	122.48	118.94
24	r	601	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
23	s	607	CHL	C4A-NA-C1A	2.30	107.74	106.71
25	S	614	LUT	C12-C13-C14	2.30	122.48	118.94
27	b	622	LHG	C20-C19-C18	-2.30	102.73	114.42
30	d	405	LMG	O2-C2-C1	-2.30	104.45	110.05
29	b	601	BCR	C3-C4-C5	-2.30	109.96	114.08
29	b	601	BCR	C27-C26-C25	2.30	126.08	122.73
23	A2	607	CHL	CHC-C4B-NB	-2.30	121.82	124.26
24	c	508	CLA	CHC-C4B-NB	2.30	126.70	124.26
29	Av	101	BCR	C15-C16-C17	-2.30	118.75	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	401	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
23	Au	605	CHL	O2D-CGD-O1D	-2.30	119.33	123.84
23	N	601	CHL	C2A-C1A-CHA	-2.30	119.83	123.86
29	h	101	BCR	C15-C16-C17	-2.30	118.76	123.47
24	Au	604	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
31	BG	403	PL9	C27-C28-C29	-2.30	122.12	127.66
24	5	613	CLA	C3B-C4B-NB	-2.30	108.38	110.52
23	7	302	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
24	a	405	CLA	C1-C2-C3	-2.30	122.06	126.04
23	AB	305	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
30	C	519	LMG	C38-C37-C36	-2.30	102.75	114.42
33	BI	102	HEM	C4C-NC-C1C	2.30	107.60	105.35
24	n	611	CLA	C1-C2-C3	-2.30	122.07	126.04
32	Az	101	SQD	C45-O47-C7	-2.30	112.13	117.79
24	v	614	CLA	C3B-C4B-NB	-2.30	108.38	110.52
23	7	310	CHL	C2D-C1D-ND	2.30	111.80	110.10
24	6	610	CLA	C2D-C1D-ND	-2.30	108.41	110.10
23	5	609	CHL	CHC-C1C-NC	-2.30	120.72	124.20
23	N	606	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
24	B	606	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
25	s	615	LUT	C12-C13-C14	2.30	122.47	118.94
27	Y	319	LHG	C20-C19-C18	-2.30	102.76	114.42
23	5	609	CHL	C2D-C1D-ND	2.30	111.80	110.10
23	A2	608	CHL	C1D-ND-C4D	-2.30	104.70	106.33
23	S	607	CHL	CHC-C4B-NB	-2.30	121.83	124.26
28	r	616	XAT	C5-C4-C3	-2.30	108.21	112.75
23	AB	306	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
24	Au	614	CLA	O2D-CGD-CBD	2.30	115.35	111.27
31	D	403	PL9	O2-C1-C6	2.30	124.56	120.59
24	n	612	CLA	C3B-C4B-NB	-2.29	108.39	110.52
38	a	409	PHO	C1C-C2C-C3C	-2.29	106.70	108.61
23	s	605	CHL	C2A-C1A-CHA	-2.29	119.85	123.86
29	8	313	BCR	C27-C26-C25	2.29	126.06	122.73
24	AB	310	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
24	AA	311	CLA	C1-C2-C3	-2.29	123.04	126.75
27	Ba	319	LHG	C20-C19-C18	-2.29	102.78	114.42
29	8	313	BCR	C15-C14-C13	-2.29	124.04	127.31
27	0	617	LHG	C5-O7-C7	-2.29	112.14	117.79
24	BV	608	CLA	CHB-C4A-NA	2.29	127.68	124.51
38	A	409	PHO	C1-C2-C3	-2.29	122.08	126.04
25	Ba	316	LUT	C39-C29-C28	2.29	121.69	118.08
27	BF	521	LHG	C18-C17-C16	-2.29	102.79	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BE	622	LHG	C20-C19-C18	-2.29	102.79	114.42
30	BG	405	LMG	O2-C2-C1	-2.29	104.48	110.05
28	BU	616	XAT	C25-C24-C23	-2.29	108.22	112.75
30	b	621	LMG	O3-C3-C2	-2.29	105.05	110.35
24	BB	312	CLA	O1D-CGD-CBD	2.29	129.17	124.48
23	BB	308	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
29	h	101	BCR	C38-C26-C25	-2.29	121.96	124.53
29	Av	101	BCR	C11-C10-C9	-2.29	124.04	127.31
29	Ay	102	BCR	C11-C10-C9	-2.29	124.04	127.31
25	5	615	LUT	C7-C8-C9	2.29	129.69	126.23
23	AB	304	CHL	C4D-CHA-C1A	-2.29	118.47	121.25
25	BV	614	LUT	C19-C9-C8	2.29	121.68	118.08
23	7	307	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
23	G	606	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
24	BF	510	CLA	CHC-C4B-NB	2.29	126.68	124.26
30	BG	405	LMG	O3-C3-C2	-2.29	105.06	110.35
30	1	519	LMG	C38-C37-C36	-2.29	102.82	114.42
24	A	406	CLA	C2D-C1D-ND	-2.29	108.42	110.10
24	C	509	CLA	C1-C2-C3	-2.29	122.09	126.04
34	1	517	DGD	CBB-CAB-C9B	-2.28	102.83	114.42
27	A2	618	LHG	C18-C17-C16	-2.28	102.83	114.42
27	BB	319	LHG	C11-C10-C9	-2.28	102.83	114.42
30	A	412	LMG	C38-C37-C36	-2.28	102.83	114.42
27	5	618	LHG	C11-C10-C9	-2.28	102.83	114.42
23	y	307	CHL	C4D-CHA-C1A	-2.28	118.47	121.25
23	Ba	310	CHL	CHD-C1D-C2D	2.28	130.27	125.48
23	r	613	CHL	CHB-C4A-NA	2.28	127.67	124.51
24	5	611	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
29	H	101	BCR	C15-C16-C17	-2.28	118.80	123.47
24	I	102	CLA	CHB-C1B-NB	2.28	126.67	124.26
25	Ba	317	LUT	C19-C9-C8	2.28	121.67	118.08
31	2	404	PL9	C37-C38-C39	-2.28	122.16	127.66
25	9	616	LUT	C35-C15-C14	2.28	128.15	123.47
38	BD	408	PHO	C1C-C2C-C3C	-2.28	106.71	108.61
29	B	619	BCR	C27-C26-C25	2.28	126.04	122.73
29	v	619	BCR	C27-C26-C25	2.28	126.04	122.73
23	G	609	CHL	C6-C5-C3	-2.28	110.89	114.62
29	BF	516	BCR	C38-C26-C25	-2.28	121.97	124.53
24	A2	614	CLA	CHB-C1B-NB	2.28	126.67	124.26
34	BF	518	DGD	C3G-C2G-C1G	-2.28	106.39	111.79
23	A2	608	CHL	O2A-CGA-CBA	2.28	119.06	111.91
34	BK	102	DGD	O5D-C6D-C5D	-2.28	104.83	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N	618	LHG	C27-C26-C25	-2.28	102.86	114.42
29	BN	101	BCR	C27-C26-C25	2.28	126.04	122.73
24	G	614	CLA	O2D-CGD-CBD	2.28	115.31	111.27
24	1	502	CLA	CHB-C1B-NB	2.28	126.67	124.26
24	6	613	CLA	C2D-C1D-ND	-2.28	108.43	110.10
29	BD	411	BCR	C15-C16-C17	-2.28	118.81	123.47
30	BE	621	LMG	O3-C3-C2	-2.28	105.09	110.35
29	BE	601	BCR	C3-C4-C5	-2.28	110.01	114.08
30	B	624	LMG	C40-C39-C38	-2.28	102.87	114.42
24	BE	609	CLA	CHC-C4B-NB	2.28	126.67	124.26
24	1	507	CLA	CHC-C4B-NB	2.28	126.67	124.26
30	v	623	LMG	C40-C39-C38	-2.28	102.87	114.42
24	b	605	CLA	C3B-C4B-NB	-2.28	108.40	110.52
24	AB	308	CLA	O2D-CGD-CBD	2.28	115.31	111.27
23	N	607	CHL	CHC-C4B-NB	-2.27	121.85	124.26
30	A0	201	LMG	C38-C37-C36	-2.27	102.88	114.42
27	r	618	LHG	C5-O7-C7	-2.27	112.19	117.79
34	BK	102	DGD	C1D-C2D-C3D	-2.27	105.26	110.00
23	A2	601	CHL	C2A-C1A-CHA	-2.27	119.88	123.86
27	n	618	LHG	C27-C26-C25	-2.27	102.88	114.42
29	BE	601	BCR	C15-C14-C13	-2.27	124.06	127.31
24	Y	311	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	0	602	CLA	CHB-C1B-NB	2.27	126.66	124.26
23	y	307	CHL	C1D-ND-C4D	-2.27	104.72	106.33
29	b	601	BCR	C15-C16-C17	-2.27	118.82	123.47
24	BJ	613	CLA	C1-C2-C3	-2.27	122.11	126.04
24	y	312	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	0	607	CHL	CHB-C4A-NA	2.27	127.65	124.51
23	BU	613	CHL	CHB-C4A-NA	2.27	127.65	124.51
24	G	611	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	Y	308	CHL	O2D-CGD-O1D	-2.27	119.40	123.84
24	9	611	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
25	s	615	LUT	C19-C9-C8	2.27	121.66	118.08
25	y	317	LUT	C19-C9-C8	2.27	121.66	118.08
23	BJ	609	CHL	O2A-CGA-CBA	2.27	119.03	111.91
24	B	606	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	6	616	LUT	C8-C9-C10	2.27	122.42	118.94
24	S	602	CLA	CHB-C1B-NB	2.27	126.66	124.26
24	C	502	CLA	CHB-C1B-NB	2.27	126.66	124.26
30	C	501	LMG	O3-C3-C2	-2.27	105.10	110.35
30	1	501	LMG	O3-C3-C2	-2.27	105.10	110.35
24	A2	613	CLA	C1-C2-C3	-2.27	122.12	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BV	607	CHL	C4A-NA-C1A	2.27	107.73	106.71
23	A2	606	CHL	C4D-CHA-C1A	-2.27	118.49	121.25
31	D	403	PL9	C37-C38-C39	-2.27	122.20	127.66
23	A2	601	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
23	6	608	CHL	C1D-ND-C4D	-2.27	104.72	106.33
29	H	101	BCR	C11-C10-C9	-2.27	124.07	127.31
25	g	616	LUT	C32-C33-C34	2.27	122.42	118.94
32	BG	406	SQD	C45-O47-C7	-2.27	112.21	117.79
24	BU	602	CLA	CMC-C2C-C1C	2.27	128.49	125.04
24	n	610	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	s	614	LUT	C19-C9-C8	2.27	121.65	118.08
23	0	608	CHL	C1D-ND-C4D	-2.27	104.72	106.33
24	BU	601	CLA	CAC-C3C-C4C	2.27	127.75	124.81
23	Ba	309	CHL	C1C-C2C-C3C	-2.27	105.32	107.11
27	BQ	618	LHG	C27-C26-C25	-2.27	102.92	114.42
23	n	609	CHL	O2A-CGA-CBA	2.27	119.02	111.91
30	d	405	LMG	O3-C3-C2	-2.27	105.11	110.35
25	A2	615	LUT	C39-C29-C28	2.26	121.64	118.08
24	n	614	CLA	CHB-C1B-NB	2.26	126.65	124.26
24	C	507	CLA	CHC-C4B-NB	2.26	126.65	124.26
23	BQ	609	CHL	O2A-CGA-CBA	2.26	119.01	111.91
23	Ba	310	CHL	C2D-C1D-ND	2.26	111.77	110.10
23	Au	606	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
24	BE	607	CLA	CHB-C1B-NB	2.26	126.65	124.26
29	BK	101	BCR	C3-C4-C5	-2.26	110.04	114.08
23	Au	608	CHL	CHC-C4B-NB	-2.26	121.86	124.26
38	BD	409	PHO	C1C-C2C-C3C	-2.26	106.73	108.61
24	Au	602	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
23	n	608	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
27	BB	319	LHG	C20-C19-C18	-2.26	102.94	114.42
23	6	609	CHL	C1D-CHD-C4C	-2.26	121.18	126.06
24	N	610	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	BB	302	CHL	OMC-CMC-C2C	-2.26	120.57	125.69
23	G	609	CHL	CHC-C1C-NC	-2.26	120.77	124.20
24	BF	506	CLA	C2D-C1D-ND	-2.26	108.44	110.10
24	B	614	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	H	101	BCR	C38-C26-C25	-2.26	121.99	124.53
29	Av	101	BCR	C2-C1-C6	2.26	113.96	110.48
23	BJ	609	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
24	9	604	CLA	C2D-C1D-ND	-2.26	108.44	110.10
27	b	623	LHG	C27-C26-C25	-2.26	102.96	114.42
24	Y	312	CLA	C1-C2-C3	-2.26	122.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	504	CLA	C1-C2-C3	-2.26	122.14	126.04
25	0	615	LUT	C32-C33-C34	2.26	122.41	118.94
24	1	509	CLA	CHC-C4B-NB	2.26	126.65	124.26
24	BF	508	CLA	CHC-C4B-NB	2.26	126.65	124.26
25	BQ	615	LUT	C39-C29-C28	2.26	121.64	118.08
24	6	610	CLA	CHC-C1C-NC	2.26	127.63	124.20
30	c	501	LMG	C38-C37-C36	-2.26	102.96	114.42
24	5	613	CLA	C1-C2-C3	-2.26	122.14	126.04
23	9	605	CHL	CHC-C4B-NB	-2.26	121.87	124.26
25	6	615	LUT	C8-C9-C10	2.26	122.41	118.94
24	BV	611	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	B	611	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
23	5	605	CHL	CHC-C4B-NB	-2.26	121.87	124.26
29	Av	101	BCR	C7-C8-C9	-2.26	122.83	126.23
23	Au	608	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
24	v	611	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
24	Ba	312	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	BE	606	CLA	C2D-C1D-ND	-2.26	108.44	110.10
34	C	517	DGD	CBB-CAB-C9B	-2.26	102.98	114.42
27	9	618	LHG	C11-C10-C9	-2.25	102.98	114.42
24	BJ	610	CLA	CHD-C1D-ND	-2.25	122.38	124.45
27	N	618	LHG	C18-C17-C16	-2.25	102.98	114.42
23	BJ	606	CHL	C4D-CHA-C1A	-2.25	118.51	121.25
24	BB	312	CLA	CHB-C1B-NB	2.25	126.64	124.26
30	B	620	LMG	O3-C3-C2	-2.25	105.14	110.35
29	b	601	BCR	C15-C14-C13	-2.25	124.09	127.31
38	R	407	PHO	CMB-C2B-C3B	2.25	128.89	124.68
24	s	608	CLA	CHB-C4A-NA	2.25	127.62	124.51
24	C	511	CLA	CHB-C1B-NB	2.25	126.64	124.26
34	H	102	DGD	O2D-C2D-C1D	-2.25	104.58	110.05
30	Aw	101	LMG	O2-C2-C1	-2.25	104.58	110.05
24	b	607	CLA	CHB-C1B-NB	2.25	126.64	124.26
23	N	601	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
27	y	319	LHG	C18-C17-C16	-2.25	103.01	114.42
24	A2	610	CLA	CHB-C4A-NA	2.25	127.62	124.51
34	BD	401	DGD	CBB-CAB-C9B	-2.25	103.02	114.42
24	BF	507	CLA	CHB-C1B-NB	2.25	126.64	124.26
23	5	607	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
27	6	617	LHG	C5-O7-C7	-2.25	112.26	117.79
34	C	518	DGD	C3D-C4D-C5D	-2.25	106.23	110.24
34	Av	102	DGD	O2D-C2D-C1D	-2.25	104.59	110.05
23	N	608	CHL	C1D-ND-C4D	-2.25	104.74	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A	408	PHO	CMB-C2B-C3B	2.25	128.88	124.68
34	1	518	DGD	C3D-C4D-C5D	-2.25	106.23	110.24
24	A2	604	CLA	C3B-C4B-NB	-2.25	108.43	110.52
23	6	601	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
23	Ba	307	CHL	C4D-CHA-C1A	-2.24	118.52	121.25
24	g	610	CLA	CHD-C1D-ND	-2.24	122.39	124.45
25	Y	316	LUT	C19-C9-C8	2.24	121.61	118.08
23	Ba	306	CHL	C4D-CHA-C1A	-2.24	118.52	121.25
23	g	609	CHL	O2A-CGA-CBA	2.24	118.95	111.91
23	n	608	CHL	O2A-CGA-CBA	2.24	118.94	111.91
24	BQ	614	CLA	CHB-C1B-NB	2.24	126.63	124.26
24	AA	304	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
29	BK	101	BCR	C15-C16-C17	-2.24	118.88	123.47
30	BF	501	LMG	C38-C37-C36	-2.24	103.04	114.42
24	0	602	CLA	C2D-C1D-ND	-2.24	108.45	110.10
25	N	616	LUT	C39-C29-C28	2.24	121.61	118.08
24	BE	609	CLA	O2D-CGD-CBD	2.24	115.25	111.27
24	BD	407	CLA	O2D-CGD-CBD	2.24	115.25	111.27
23	A2	605	CHL	C2A-C1A-CHA	-2.24	119.94	123.86
30	BF	501	LMG	C1-O6-C5	-2.24	109.29	113.69
27	v	621	LHG	C27-C26-C25	-2.24	103.06	114.42
24	5	610	CLA	CHD-C1D-ND	-2.24	122.40	124.45
24	v	616	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	A2	616	LUT	C39-C29-C28	2.24	121.60	118.08
24	7	304	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	y	309	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
30	b	621	LMG	O2-C2-C1	-2.24	104.61	110.05
25	BB	316	LUT	C39-C29-C28	2.24	121.60	118.08
27	Au	618	LHG	C18-C17-C16	-2.24	103.07	114.42
27	BE	623	LHG	C27-C26-C25	-2.24	103.07	114.42
23	8	307	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
27	B	621	LHG	C27-C26-C25	-2.24	103.08	114.42
31	2	404	PL9	C20-C19-C21	2.24	119.03	115.27
29	AB	313	BCR	C35-C13-C14	-2.24	119.79	122.92
32	L	101	SQD	C45-O47-C7	-2.23	112.29	117.79
23	8	307	CHL	CHB-C4A-NA	2.23	127.60	124.51
34	h	102	DGD	CBB-CAB-C9B	-2.23	103.08	114.42
24	a	407	CLA	CHB-C1B-NB	2.23	126.62	124.26
27	y	319	LHG	C27-C26-C25	-2.23	103.08	114.42
24	BE	611	CLA	C2D-C1D-ND	-2.23	108.46	110.10
25	AA	316	LUT	C39-C29-C28	2.23	121.60	118.08
27	Az	102	LHG	C18-C17-C16	-2.23	103.09	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Ba	319	LHG	C27-C26-C25	-2.23	103.09	114.42
24	C	511	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
24	Ba	312	CLA	C1-C2-C3	-2.23	122.18	126.04
29	BE	601	BCR	C15-C16-C17	-2.23	118.90	123.47
30	D	405	LMG	O1-C1-C2	-2.23	104.82	108.30
34	a	401	DGD	CBB-CAB-C9B	-2.23	103.09	114.42
24	R	406	CLA	CGD-CBD-CAD	2.23	117.96	110.73
24	G	604	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
24	Au	602	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
29	v	619	BCR	C15-C16-C17	-2.23	118.90	123.47
24	G	602	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
25	7	317	LUT	C32-C33-C34	2.23	122.36	118.94
24	A	407	CLA	CGD-CBD-CAD	2.23	117.96	110.73
24	9	613	CLA	C3B-C4B-NB	-2.23	108.45	110.52
24	Au	613	CLA	C3B-C4B-NB	-2.23	108.45	110.52
24	9	614	CLA	CHB-C1B-NB	2.23	126.62	124.26
24	G	602	CLA	C1-C2-C3	-2.23	122.19	126.04
23	y	306	CHL	C4D-CHA-C1A	-2.23	118.53	121.25
24	s	611	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
24	0	610	CLA	CHD-C1D-ND	-2.23	122.41	124.45
27	Ba	319	LHG	C18-C17-C16	-2.23	103.11	114.42
24	N	604	CLA	C3B-C4B-NB	-2.23	108.45	110.52
23	9	609	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
23	G	608	CHL	CHC-C4B-NB	-2.23	121.90	124.26
24	AA	311	CLA	CHB-C1B-NB	2.23	126.62	124.26
24	BB	313	CLA	CHB-C1B-NB	2.23	126.62	124.26
27	9	618	LHG	C18-C17-C16	-2.23	103.11	114.42
27	G	618	LHG	C18-C17-C16	-2.23	103.11	114.42
29	k	101	BCR	C15-C16-C17	-2.23	118.91	123.47
30	v	620	LMG	O3-C3-C2	-2.23	105.20	110.35
23	N	608	CHL	O2A-CGA-CBA	2.23	118.89	111.91
24	b	609	CLA	O2D-CGD-CBD	2.23	115.22	111.27
29	4	101	BCR	C7-C8-C9	-2.23	122.87	126.23
23	6	601	CHL	C1C-C2C-C3C	-2.23	105.35	107.11
23	Ba	307	CHL	CHC-C4B-NB	-2.23	121.90	124.26
30	Aw	101	LMG	C40-C39-C38	-2.23	103.13	114.42
23	0	607	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
24	r	614	CLA	C3B-C4B-NB	-2.22	108.45	110.52
24	1	506	CLA	C1-C2-C3	-2.22	122.20	126.04
24	6	613	CLA	CHC-C4B-NB	2.22	126.61	124.26
23	BJ	605	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
27	BU	617	LHG	C18-C17-C16	-2.22	103.14	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	609	CHL	CHD-C1D-C2D	2.22	130.14	125.48
24	BF	510	CLA	C1-C2-C3	-2.22	122.20	126.04
29	Ay	101	BCR	C2-C1-C6	2.22	113.90	110.48
24	n	610	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
29	BK	101	BCR	C38-C26-C25	-2.22	122.03	124.53
23	BU	606	CHL	CHC-C4B-NB	-2.22	121.91	124.26
28	r	616	XAT	C25-C24-C23	-2.22	108.36	112.75
38	R	407	PHO	C2D-C1D-ND	-2.22	107.99	109.53
25	y	316	LUT	C39-C29-C28	2.22	121.58	118.08
30	I	101	LMG	C40-C39-C38	-2.22	103.16	114.42
23	Y	308	CHL	C6-C5-C3	-2.22	110.99	114.62
24	BE	613	CLA	CHC-C4B-NB	2.22	126.61	124.26
27	c	519	LHG	C27-C26-C25	-2.22	103.16	114.42
23	6	605	CHL	C4D-CHA-C1A	-2.22	118.55	121.25
28	N	619	XAT	C5-C4-C3	-2.22	108.36	112.75
24	BB	315	CLA	CHB-C1B-NB	2.22	126.61	124.26
24	BB	313	CLA	C2D-C1D-ND	-2.22	108.47	110.10
24	BV	604	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
34	BK	102	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
27	v	621	LHG	C20-C19-C18	-2.22	103.16	114.42
24	Y	312	CLA	CHB-C1B-NB	2.22	126.61	124.26
23	7	302	CHL	C4A-NA-C1A	2.22	107.70	106.71
24	BB	312	CLA	C1-C2-C3	-2.22	122.21	126.04
29	BN	101	BCR	C15-C16-C17	-2.22	118.93	123.47
34	1	516	DGD	CAB-C9B-C8B	-2.22	103.17	114.42
29	k	101	BCR	C15-C14-C13	-2.22	124.15	127.31
28	A2	619	XAT	C5-C4-C3	-2.22	108.37	112.75
25	G	615	LUT	C31-C30-C29	2.21	130.47	127.31
28	BU	616	XAT	C4-C3-C2	-2.21	106.50	110.77
23	0	605	CHL	C4D-CHA-C1A	-2.21	118.55	121.25
24	C	511	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
29	4	101	BCR	C16-C15-C14	-2.21	118.94	123.47
27	w	201	LHG	C20-C19-C18	-2.21	103.19	114.42
24	N	602	CLA	CHB-C1B-NB	2.21	126.60	124.26
25	BV	615	LUT	C19-C9-C8	2.21	121.56	118.08
27	n	618	LHG	C18-C17-C16	-2.21	103.19	114.42
23	g	606	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
23	A2	607	CHL	CED-O2D-CGD	2.21	120.94	115.94
30	BE	621	LMG	O2-C2-C1	-2.21	104.67	110.05
27	BF	520	LHG	C27-C26-C25	-2.21	103.19	114.42
23	y	310	CHL	C2D-C1D-ND	2.21	111.73	110.10
24	5	604	CLA	C2D-C1D-ND	-2.21	108.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ba	307	CHL	C1D-ND-C4D	-2.21	104.76	106.33
23	9	608	CHL	CHC-C4B-NB	-2.21	121.92	124.26
27	r	618	LHG	C18-C17-C16	-2.21	103.20	114.42
27	6	617	LHG	C27-C26-C25	-2.21	103.20	114.42
25	BJ	616	LUT	C32-C33-C34	2.21	122.33	118.94
23	r	606	CHL	CHC-C4B-NB	-2.21	121.92	124.26
27	BF	521	LHG	C27-C26-C25	-2.21	103.21	114.42
27	BQ	618	LHG	C18-C17-C16	-2.21	103.21	114.42
31	D	403	PL9	C20-C19-C21	2.21	118.99	115.27
29	AB	313	BCR	C15-C14-C13	-2.21	124.16	127.31
24	BB	304	CLA	CHB-C1B-NB	2.21	126.59	124.26
27	W	201	LHG	C20-C19-C18	-2.21	103.21	114.42
29	k	101	BCR	C27-C26-C25	2.21	125.94	122.73
27	BY	201	LHG	C20-C19-C18	-2.21	103.22	114.42
24	BF	512	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
27	B	621	LHG	C20-C19-C18	-2.21	103.22	114.42
23	N	607	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
24	7	313	CLA	CHB-C1B-NB	2.21	126.59	124.26
30	Aw	101	LMG	O1-C7-C8	-2.21	105.58	110.90
23	BQ	607	CHL	C2A-C1A-CHA	-2.21	120.00	123.86
29	Av	101	BCR	C38-C26-C25	-2.21	122.05	124.53
24	9	603	CLA	CHB-C1B-NB	2.21	126.59	124.26
29	BI	101	BCR	C16-C15-C14	-2.21	118.96	123.47
30	d	405	LMG	O1-C1-C2	-2.21	104.86	108.30
25	Y	316	LUT	C39-C29-C28	2.20	121.55	118.08
24	G	613	CLA	C3B-C4B-NB	-2.20	108.47	110.52
24	BE	613	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
27	0	617	LHG	C27-C26-C25	-2.20	103.24	114.42
24	5	614	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	Au	615	LUT	C31-C30-C29	2.20	130.46	127.31
24	6	604	CLA	CHD-C1D-ND	-2.20	122.43	124.45
27	5	618	LHG	C18-C17-C16	-2.20	103.24	114.42
24	B	615	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
27	Y	319	LHG	C27-C26-C25	-2.20	103.24	114.42
23	BQ	608	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
29	Ay	101	BCR	C15-C16-C17	-2.20	118.96	123.47
24	C	506	CLA	C1-C2-C3	-2.20	122.23	126.04
24	9	613	CLA	C1-C2-C3	-2.20	122.23	126.04
23	g	609	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
23	Au	607	CHL	CHC-C4B-NB	-2.20	121.93	124.26
23	y	310	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
23	A2	607	CHL	C1C-C2C-C3C	-2.20	105.37	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	319	LHG	C27-C26-C25	-2.20	103.25	114.42
23	N	601	CHL	CHB-C4A-NA	2.20	127.56	124.51
23	BU	613	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
34	C	516	DGD	CAB-C9B-C8B	-2.20	103.25	114.42
25	A6	615	LUT	C32-C33-C34	2.20	122.32	118.94
23	g	607	CHL	C6-C5-C3	-2.20	111.02	114.62
23	0	601	CHL	OMC-CMC-C2C	-2.20	120.71	125.69
23	A6	607	CHL	C3B-C4B-NB	2.20	112.56	110.52
23	G	609	CHL	CHD-C1D-C2D	2.20	130.09	125.48
23	N	607	CHL	CED-O2D-CGD	2.20	120.91	115.94
30	v	623	LMG	O2-C2-C1	-2.20	104.71	110.05
24	BU	604	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
27	BE	624	LHG	C18-C17-C16	-2.20	103.27	114.42
24	BF	506	CLA	O2D-CGD-CBD	2.20	115.17	111.27
34	Av	102	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
24	A2	604	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
34	H	102	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
27	c	520	LHG	C27-C26-C25	-2.20	103.28	114.42
30	BG	405	LMG	O1-C1-C2	-2.20	104.88	108.30
27	c	519	LHG	C18-C17-C16	-2.19	103.28	114.42
24	BE	617	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
34	H	102	DGD	O5D-C6D-C5D	-2.19	104.99	109.05
31	BG	403	PL9	C37-C38-C39	-2.19	122.38	127.66
24	BJ	611	CLA	O2D-CGD-CBD	2.19	115.17	111.27
23	0	609	CHL	CBC-CAC-C3C	-2.19	106.38	112.43
23	y	309	CHL	C1D-ND-C4D	-2.19	104.78	106.33
25	BV	614	LUT	C31-C30-C29	2.19	130.44	127.31
27	b	622	LHG	C27-C26-C25	-2.19	103.30	114.42
23	BQ	608	CHL	O2A-CGA-CBA	2.19	118.79	111.91
23	BJ	607	CHL	C6-C5-C3	-2.19	111.03	114.62
25	AA	316	LUT	C8-C9-C10	2.19	122.30	118.94
24	b	613	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
29	BE	618	BCR	C7-C8-C9	-2.19	122.92	126.23
24	6	604	CLA	CHC-C4B-NB	2.19	126.58	124.26
23	y	302	CHL	C4-C3-C5	2.19	118.95	115.27
29	f	101	BCR	C16-C15-C14	-2.19	118.99	123.47
23	Ba	306	CHL	CHC-C4B-NB	-2.19	121.94	124.26
24	y	311	CLA	CHB-C1B-NB	2.19	126.57	124.26
24	BV	610	CLA	C1-C2-C3	-2.19	122.26	126.04
23	A2	601	CHL	CHB-C4A-NA	2.19	127.54	124.51
29	v	622	BCR	C11-C10-C9	-2.19	124.19	127.31
27	A0	202	LHG	C20-C19-C18	-2.19	103.32	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BE	624	LHG	C27-C26-C25	-2.19	103.32	114.42
24	v	609	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	0	613	CLA	CHC-C4B-NB	2.19	126.57	124.26
24	v	610	CLA	CHB-C1B-NB	2.19	126.57	124.26
24	2	402	CLA	O2D-CGD-CBD	2.19	115.16	111.27
30	B	624	LMG	O2-C2-C1	-2.19	104.73	110.05
24	BV	609	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
24	BD	406	CLA	C1-C2-C3	-2.19	122.26	126.04
33	4	102	HEM	C3D-C4D-ND	-2.19	107.73	110.17
27	C	520	LHG	C18-C17-C16	-2.19	103.33	114.42
24	BB	311	CLA	C3B-C4B-NB	-2.19	108.49	110.52
23	5	606	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
34	BK	102	DGD	O2D-C2D-C1D	-2.19	104.74	110.05
27	BE	622	LHG	C27-C26-C25	-2.19	103.33	114.42
24	c	512	CLA	CGD-CBD-CAD	2.19	117.81	110.73
23	5	607	CHL	O2A-CGA-CBA	2.19	118.77	111.91
27	1	520	LHG	C18-C17-C16	-2.19	103.33	114.42
24	BE	612	CLA	C1-C2-C3	-2.18	122.26	126.04
23	BU	613	CHL	CAA-C2A-C3A	-2.18	111.00	116.10
23	y	307	CHL	CHC-C4B-NB	-2.18	121.94	124.26
23	BU	613	CHL	CMA-C3A-C2A	-2.18	111.00	116.10
38	BD	408	PHO	C2D-C1D-ND	-2.18	108.02	109.53
29	BE	619	BCR	C15-C14-C13	-2.18	124.19	127.31
24	b	609	CLA	CHC-C4B-NB	2.18	126.57	124.26
27	g	618	LHG	C27-C26-C25	-2.18	103.34	114.42
23	8	305	CHL	OMC-CMC-C2C	-2.18	120.75	125.69
23	A6	607	CHL	CHD-C1D-C2D	2.18	130.06	125.48
27	BF	520	LHG	C18-C17-C16	-2.18	103.34	114.42
23	S	605	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
23	BQ	606	CHL	C4D-CHA-C1A	-2.18	118.59	121.25
24	b	606	CLA	C2D-C1D-ND	-2.18	108.50	110.10
29	F	101	BCR	C7-C8-C9	-2.18	122.94	126.23
24	6	603	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
25	5	615	LUT	C28-C29-C30	2.18	122.29	118.94
24	g	611	CLA	O2D-CGD-CBD	2.18	115.14	111.27
38	a	408	PHO	C1C-C2C-C3C	-2.18	106.80	108.61
27	b	624	LHG	C27-C26-C25	-2.18	103.35	114.42
27	A0	202	LHG	C27-C26-C25	-2.18	103.35	114.42
24	A2	602	CLA	CHB-C1B-NB	2.18	126.57	124.26
24	A2	603	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	BQ	601	CHL	CHB-C4A-NA	2.18	127.53	124.51
23	g	601	CHL	C6-C5-C3	-2.18	111.06	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BJ	601	CHL	C6-C5-C3	-2.18	111.06	114.62
26	BB	320	NEX	C2-C1-C6	2.18	111.33	109.21
24	y	313	CLA	O2D-CGD-CBD	2.18	115.14	111.27
23	0	601	CHL	C1C-C2C-C3C	-2.18	105.39	107.11
24	9	604	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	c	501	LMG	C1-O6-C5	-2.18	109.41	113.69
29	B	619	BCR	C15-C16-C17	-2.18	119.01	123.47
23	BQ	606	CHL	O2A-CGA-O1A	-2.18	118.10	123.59
23	BU	606	CHL	C6-C5-C3	-2.18	111.06	114.62
23	5	609	CHL	C1D-CHD-C4C	-2.18	121.36	126.06
24	8	308	CLA	O2D-CGD-CBD	2.18	115.14	111.27
23	N	605	CHL	C2A-C1A-CHA	-2.18	120.05	123.86
27	BB	319	LHG	C18-C17-C16	-2.18	103.38	114.42
24	c	502	CLA	CHB-C1B-NB	2.18	126.56	124.26
31	d	403	PL9	C20-C19-C21	2.18	118.93	115.27
23	7	309	CHL	CHB-C4A-NA	2.18	127.52	124.51
25	A6	614	LUT	C31-C30-C29	2.18	130.41	127.31
24	Ba	313	CLA	O2D-CGD-CBD	2.18	115.13	111.27
34	BF	518	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
23	g	605	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
23	n	601	CHL	CHB-C4A-NA	2.17	127.52	124.51
33	F	102	HEM	C3D-C4D-ND	-2.17	107.75	110.17
29	b	620	BCR	C27-C26-C25	2.17	125.89	122.73
24	c	510	CLA	CHC-C4B-NB	2.17	126.56	124.26
29	8	313	BCR	C15-C16-C17	-2.17	119.02	123.47
24	AB	308	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
23	9	606	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
23	6	608	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
27	C	521	LHG	C27-C26-C25	-2.17	103.40	114.42
29	F	101	BCR	C16-C15-C14	-2.17	119.02	123.47
23	BQ	606	CHL	C1D-ND-C4D	-2.17	104.79	106.33
23	BQ	606	CHL	OMC-CMC-C2C	-2.17	120.78	125.69
24	BJ	602	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	y	306	CHL	CHC-C4B-NB	-2.17	121.96	124.26
24	2	403	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
30	B	620	LMG	O1-C1-C2	-2.17	104.91	108.30
23	Y	310	CHL	CHC-C4B-NB	-2.17	121.96	124.26
25	n	616	LUT	C39-C29-C28	2.17	121.50	118.08
29	BN	101	BCR	C8-C7-C6	-2.17	121.11	127.20
34	C	517	DGD	CAB-C9B-C8B	-2.17	103.41	114.42
29	z	101	BCR	C8-C7-C6	-2.17	121.11	127.20
24	A6	610	CLA	CHB-C1B-NB	2.17	126.55	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
29	BN	101	BCR	C15-C14-C13	-2.17	124.21	127.31
27	Y	319	LHG	C18-C17-C16	-2.17	103.41	114.42
24	C	509	CLA	CHC-C4B-NB	2.17	126.55	124.26
24	v	604	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
34	1	517	DGD	CAB-C9B-C8B	-2.17	103.42	114.42
24	b	605	CLA	CHD-C1D-ND	-2.17	122.46	124.45
29	C	514	BCR	C24-C23-C22	-2.17	122.96	126.23
27	W	201	LHG	C27-C26-C25	-2.17	103.42	114.42
24	a	406	CLA	C1-C2-C3	-2.17	122.30	126.04
24	A6	613	CLA	C2D-C1D-ND	-2.17	108.51	110.10
23	n	607	CHL	C2A-C1A-CHA	-2.17	120.07	123.86
24	s	609	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
31	2	404	PL9	C12-C13-C14	-2.17	122.44	127.66
27	B	622	LHG	C27-C26-C25	-2.17	103.43	114.42
23	AA	309	CHL	CHB-C4A-NA	2.17	127.51	124.51
23	9	607	CHL	C2A-C1A-CHA	-2.17	120.07	123.86
23	y	307	CHL	CAA-C2A-C1A	2.17	119.07	111.97
24	BB	315	CLA	O2D-CGD-CBD	2.17	115.12	111.27
24	BF	513	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
27	1	521	LHG	C27-C26-C25	-2.17	103.43	114.42
24	Aw	102	CLA	C1-C2-C3	-2.17	122.30	126.04
23	Y	302	CHL	OMC-CMC-C2C	-2.17	120.79	125.69
29	A	411	BCR	C11-C10-C9	-2.17	124.22	127.31
27	BJ	618	LHG	C27-C26-C25	-2.17	103.43	114.42
30	C	519	LMG	O3-C3-C2	-2.16	105.34	110.35
23	BU	605	CHL	CHC-C1C-C2C	-2.16	118.26	126.11
23	Ba	307	CHL	CAA-C2A-C1A	2.16	119.07	111.97
24	5	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
24	Ba	311	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	c	517	DGD	CBB-CAB-C9B	-2.16	103.44	114.42
23	0	601	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
27	L	102	LHG	C18-C17-C16	-2.16	103.44	114.42
23	BB	302	CHL	O2A-CGA-O1A	-2.16	118.13	123.59
24	v	610	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
25	9	616	LUT	C31-C30-C29	2.16	130.40	127.31
34	c	516	DGD	CBB-CAB-C9B	-2.16	103.45	114.42
27	g	618	LHG	C18-C17-C16	-2.16	103.45	114.42
34	c	517	DGD	CAB-C9B-C8B	-2.16	103.45	114.42
23	9	607	CHL	O2A-CGA-CBA	2.16	118.69	111.91
30	1	519	LMG	O3-C3-C2	-2.16	105.35	110.35
24	g	602	CLA	O2A-CGA-O1A	-2.16	118.14	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BV	609	CLA	C3B-C4B-NB	-2.16	108.51	110.52
24	a	407	CLA	O2D-CGD-CBD	2.16	115.11	111.27
25	BB	316	LUT	C31-C30-C29	2.16	130.39	127.31
31	D	403	PL9	C12-C13-C14	-2.16	122.46	127.66
24	b	612	CLA	C1-C2-C3	-2.16	122.31	126.04
23	5	608	CHL	CHC-C4B-NB	-2.16	121.97	124.26
24	r	609	CLA	CHB-C1B-NB	2.16	126.54	124.26
24	A6	608	CLA	CHB-C1B-NB	2.16	126.54	124.26
24	Au	614	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
25	n	616	LUT	C1-C6-C5	-2.16	119.57	122.61
24	R	404	CLA	C1-C2-C3	-2.16	122.31	126.04
34	C	518	DGD	CAB-C9B-C8B	-2.16	103.47	114.42
23	Y	306	CHL	CED-O2D-CGD	2.16	120.82	115.94
24	D	402	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
24	7	304	CLA	CHD-C1D-ND	-2.16	122.47	124.45
38	A	408	PHO	C1C-C2C-C3C	-2.16	106.82	108.61
24	BV	612	CLA	CHC-C4B-NB	2.16	126.54	124.26
23	AA	302	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
23	0	609	CHL	C1D-CHD-C4C	-2.16	121.41	126.06
23	r	607	CHL	CHC-C4B-NB	-2.16	121.97	124.26
25	BQ	616	LUT	C12-C13-C14	2.16	122.25	118.94
34	c	516	DGD	O2D-C2D-C1D	-2.16	104.81	110.05
23	N	605	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
24	b	617	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
24	6	613	CLA	CHB-C1B-NB	2.16	126.54	124.26
34	BF	517	DGD	CBB-CAB-C9B	-2.16	103.48	114.42
29	1	514	BCR	C24-C23-C22	-2.16	122.98	126.23
24	s	610	CLA	CED-O2D-CGD	2.16	120.81	115.94
24	BD	410	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
24	Au	602	CLA	C1-C2-C3	-2.15	122.32	126.04
24	y	312	CLA	C2D-C1D-ND	-2.15	108.52	110.10
24	A6	602	CLA	CHB-C1B-NB	2.15	126.54	124.26
24	BD	407	CLA	CHB-C1B-NB	2.15	126.54	124.26
27	BJ	618	LHG	C18-C17-C16	-2.15	103.49	114.42
25	9	616	LUT	C12-C13-C14	2.15	122.25	118.94
23	Y	307	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
24	BV	610	CLA	CED-O2D-CGD	2.15	120.81	115.94
29	BE	618	BCR	C39-C30-C25	2.15	113.79	110.30
25	S	615	LUT	C11-C10-C9	2.15	130.38	127.31
34	1	518	DGD	CAB-C9B-C8B	-2.15	103.50	114.42
24	B	608	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
24	v	615	CLA	O2A-CGA-O1A	-2.15	118.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	609	CHL	O2A-CGA-CBA	2.15	118.66	111.91
24	1	503	CLA	CHB-C1B-NB	2.15	126.53	124.26
23	N	606	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
23	r	605	CHL	O1D-CGD-CBD	-2.15	120.08	124.48
24	BF	510	CLA	CHB-C1B-NB	2.15	126.53	124.26
30	2	407	LMG	O1-C1-C2	-2.15	104.94	108.30
38	a	408	PHO	CMB-C2B-C3B	2.15	128.70	124.68
23	n	606	CHL	O2A-CGA-O1A	-2.15	118.16	123.59
24	I	102	CLA	C1-C2-C3	-2.15	122.32	126.04
23	AA	302	CHL	CHD-C1D-C2D	2.15	129.99	125.48
24	AA	311	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	Y	315	CLA	CHB-C1B-NB	2.15	126.53	124.26
24	B	601	CLA	O2D-CGD-CBD	2.15	115.09	111.27
34	BF	518	DGD	CAB-C9B-C8B	-2.15	103.51	114.42
32	Az	101	SQD	O6-C44-C45	-2.15	105.71	110.90
23	5	607	CHL	C2A-C1A-CHA	-2.15	120.10	123.86
29	1	514	BCR	C15-C14-C13	-2.15	124.24	127.31
23	6	601	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
24	v	611	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	S	608	CLA	CHB-C1B-NB	2.15	126.53	124.26
23	AA	302	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
30	v	620	LMG	O1-C1-C2	-2.15	104.95	108.30
24	7	311	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	Au	606	CHL	OMC-CMC-C2C	-2.15	120.83	125.69
24	Ba	314	CLA	CHC-C4B-NB	2.15	126.53	124.26
25	0	616	LUT	C8-C9-C10	2.15	122.23	118.94
23	7	307	CHL	OMC-CMC-C2C	-2.15	120.84	125.69
27	2	405	LHG	C27-C26-C25	-2.15	103.53	114.42
24	s	610	CLA	C1-C2-C3	-2.15	122.33	126.04
24	Y	312	CLA	O1D-CGD-CBD	2.15	128.87	124.48
24	y	311	CLA	CHD-C1D-ND	-2.14	122.48	124.45
24	BE	605	CLA	CHD-C1D-ND	-2.14	122.48	124.45
24	0	603	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
24	BE	611	CLA	CHB-C1B-NB	2.14	126.53	124.26
24	BU	602	CLA	CHB-C1B-NB	2.14	126.53	124.26
23	BB	307	CHL	CAA-C2A-C1A	2.14	119.00	111.97
23	r	606	CHL	CED-O2D-CGD	2.14	120.79	115.94
29	Bb	101	BCR	C8-C7-C6	-2.14	121.18	127.20
29	b	619	BCR	C15-C14-C13	-2.14	124.25	127.31
23	8	304	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
24	b	605	CLA	CHB-C1B-NB	2.14	126.53	124.26
27	Az	102	LHG	C5-O7-C7	-2.14	112.52	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Y	306	CHL	C4A-NA-C1A	2.14	107.67	106.71
23	BU	613	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
24	6	604	CLA	CHD-C4C-C3C	-2.14	121.69	124.84
34	C	516	DGD	CBB-CAB-C9B	-2.14	103.56	114.42
29	v	622	BCR	C7-C8-C9	-2.14	123.00	126.23
24	A6	613	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
34	1	516	DGD	C1D-C2D-C3D	-2.14	105.54	110.00
24	Ba	313	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	AA	305	CLA	CHD-C1D-ND	-2.14	122.49	124.45
34	c	516	DGD	O3E-C3E-C2E	-2.14	105.40	110.35
31	BG	403	PL9	C20-C19-C21	2.14	118.87	115.27
23	BV	607	CHL	C1C-C2C-C3C	-2.14	105.42	107.11
24	BF	502	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	g	616	LUT	C11-C12-C13	2.14	132.43	126.42
24	1	512	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	BB	308	CHL	C6-C5-C3	-2.14	111.12	114.62
25	6	615	LUT	C12-C13-C14	2.14	122.22	118.94
24	v	605	CLA	C2D-C1D-ND	-2.14	108.53	110.10
23	BU	607	CHL	CHC-C4B-NB	-2.14	121.99	124.26
24	r	610	CLA	CHB-C1B-NB	2.14	126.52	124.26
29	B	623	BCR	C11-C10-C9	-2.14	124.26	127.31
25	AA	317	LUT	C8-C9-C10	2.14	122.22	118.94
23	A2	606	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
23	A6	605	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
24	AA	305	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
23	G	606	CHL	OMC-CMC-C2C	-2.14	120.85	125.69
24	Y	313	CLA	C2D-C1D-ND	-2.14	108.53	110.10
24	A6	602	CLA	C2D-C1D-ND	-2.14	108.53	110.10
23	6	607	CHL	CHB-C4A-NA	2.14	127.47	124.51
34	a	413	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
24	y	314	CLA	CHC-C4B-NB	2.14	126.52	124.26
29	BE	620	BCR	C27-C26-C25	2.14	125.83	122.73
24	BF	502	CLA	C2D-C1D-ND	-2.14	108.53	110.10
24	AB	310	CLA	CHB-C1B-NB	2.14	126.52	124.26
30	C	501	LMG	O2-C2-C1	-2.14	104.86	110.05
29	B	623	BCR	C7-C8-C9	-2.14	123.01	126.23
27	L	102	LHG	C27-C26-C25	-2.14	103.58	114.42
24	7	305	CLA	CMB-C2B-C1B	-2.14	122.12	125.37
29	H	101	BCR	C15-C14-C13	-2.13	124.26	127.31
34	BF	517	DGD	CAB-C9B-C8B	-2.13	103.59	114.42
24	N	611	CLA	O2D-CGD-CBD	2.13	115.06	111.27
24	Ba	312	CLA	C2D-C1D-ND	-2.13	108.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BD	413	DGD	CAB-C9B-C8B	-2.13	103.59	114.42
24	N	603	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	N	604	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	A2	611	CLA	O2D-CGD-CBD	2.13	115.06	111.27
24	Ba	311	CLA	CHB-C1B-NB	2.13	126.52	124.26
29	BF	515	BCR	C8-C7-C6	-2.13	121.21	127.20
23	n	609	CHL	C6-C5-C3	-2.13	111.13	114.62
23	G	607	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
34	Av	102	DGD	O5D-C6D-C5D	-2.13	105.10	109.05
34	1	518	DGD	CBB-CAB-C9B	-2.13	103.59	114.42
24	C	512	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
34	h	102	DGD	O2D-C2D-C1D	-2.13	104.86	110.05
24	B	605	CLA	C2D-C1D-ND	-2.13	108.53	110.10
24	6	614	CLA	CHB-C1B-NB	2.13	126.52	124.26
34	c	516	DGD	CAB-C9B-C8B	-2.13	103.60	114.42
24	S	612	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
24	c	510	CLA	C1-C2-C3	-2.13	122.36	126.04
24	BU	614	CLA	C2D-C1D-ND	-2.13	108.53	110.10
27	BY	201	LHG	C27-C26-C25	-2.13	103.60	114.42
24	G	614	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	AB	310	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	AA	307	CHL	CED-O2D-CGD	2.13	120.76	115.94
24	v	601	CLA	O2D-CGD-CBD	2.13	115.06	111.27
23	y	307	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
23	0	608	CHL	O2D-CGD-O1D	-2.13	119.67	123.84
24	8	310	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	5	615	LUT	C35-C34-C33	2.13	130.35	127.31
24	C	503	CLA	CHB-C1B-NB	2.13	126.51	124.26
24	5	613	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
23	A6	601	CHL	O1D-CGD-CBD	-2.13	120.13	124.48
34	C	518	DGD	CBB-CAB-C9B	-2.13	103.61	114.42
24	B	616	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	AA	304	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	8	308	CLA	CAC-C3C-C4C	2.13	127.57	124.81
32	BO	102	SQD	C45-O47-C7	-2.13	112.55	117.79
23	0	607	CHL	C2A-C1A-CHA	-2.13	120.14	123.86
24	9	603	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	5	603	CLA	C1-C2-C3	-2.13	122.36	126.04
23	s	607	CHL	C4D-CHA-C1A	-2.13	118.66	121.25
29	z	102	BCR	C8-C7-C6	-2.13	121.23	127.20
34	BF	517	DGD	O3E-C3E-C2E	-2.13	105.43	110.35
23	6	608	CHL	C4D-CHA-C1A	-2.13	118.66	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	607	CHL	CHC-C4B-NB	-2.13	122.00	124.26
25	BQ	616	LUT	C39-C29-C28	2.13	121.43	118.08
24	Y	305	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
27	Az	102	LHG	C27-C26-C25	-2.13	103.63	114.42
23	Ba	302	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
23	AB	307	CHL	C2D-C1D-ND	2.13	111.67	110.10
25	s	615	LUT	C1-C6-C5	-2.13	119.62	122.61
23	s	607	CHL	C1C-C2C-C3C	-2.13	105.43	107.11
29	C	514	BCR	C15-C16-C17	-2.13	119.12	123.47
24	r	603	CLA	CHB-C1B-NB	2.13	126.51	124.26
23	7	302	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
24	b	611	CLA	CHC-C1C-NC	2.13	127.43	124.20
24	r	614	CLA	C2D-C1D-ND	-2.13	108.54	110.10
24	A6	609	CLA	C2D-C1D-ND	-2.13	108.54	110.10
25	S	615	LUT	C32-C33-C34	2.12	122.20	118.94
24	6	603	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
30	c	501	LMG	O2-C2-C1	-2.12	104.89	110.05
23	y	309	CHL	O2A-CGA-CBA	2.12	118.57	111.91
23	BB	307	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
24	1	512	CLA	CHB-C1B-NB	2.12	126.50	124.26
34	h	102	DGD	O5D-C6D-C5D	-2.12	105.12	109.05
24	A	405	CLA	C1-C2-C3	-2.12	122.37	126.04
23	BV	607	CHL	CED-O2D-CGD	2.12	120.74	115.94
23	8	307	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
24	7	305	CLA	CHD-C1D-ND	-2.12	122.50	124.45
24	BE	605	CLA	CHB-C1B-NB	2.12	126.50	124.26
23	BV	607	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
24	BE	616	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	A2	607	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
24	BQ	614	CLA	CED-O2D-CGD	2.12	120.74	115.94
24	B	610	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	BB	315	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
23	5	609	CHL	C3B-C4B-NB	2.12	112.48	110.52
30	1	501	LMG	O2-C2-C1	-2.12	104.89	110.05
23	AA	307	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
24	0	610	CLA	CMA-C3A-C2A	-2.12	105.27	113.83
24	BU	608	CLA	O2D-CGD-CBD	2.12	115.04	111.27
25	Y	316	LUT	C31-C30-C29	2.12	130.34	127.31
24	S	610	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	n	603	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	A2	610	CLA	O2D-CGD-CBD	2.12	115.03	111.27
24	A	406	CLA	CHD-C1D-C2D	2.12	129.93	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	520	LHG	C27-C26-C25	-2.12	103.66	114.42
24	Au	612	CLA	CHB-C1B-NB	2.12	126.50	124.26
23	BQ	609	CHL	C6-C5-C3	-2.12	111.15	114.62
24	v	613	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	A	405	CLA	O2D-CGD-CBD	2.12	115.03	111.27
29	C	514	BCR	C15-C14-C13	-2.12	124.29	127.31
23	9	609	CHL	O2A-CGA-CBA	2.12	118.55	111.91
25	BB	316	LUT	C19-C9-C8	2.12	121.41	118.08
24	BB	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	BU	606	CHL	CED-O2D-CGD	2.12	120.73	115.94
24	5	603	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
34	C	518	DGD	O2D-C2D-C1D	-2.12	104.90	110.05
24	B	609	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	BB	308	CHL	OMC-CMC-C2C	-2.12	120.90	125.69
23	e	601	CHL	O2D-CGD-O1D	-2.12	119.28	124.09
23	BU	606	CHL	C1D-CHD-C4C	-2.12	121.49	126.06
29	BD	411	BCR	C15-C14-C13	-2.12	124.29	127.31
24	Y	313	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	s	612	CLA	CHC-C4B-NB	2.12	126.50	124.26
23	Ba	309	CHL	O2A-CGA-CBA	2.12	118.55	111.91
34	BF	517	DGD	C1D-C2D-C3D	-2.12	105.59	110.00
24	S	613	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	n	609	CHL	C4A-NA-C1A	2.12	107.66	106.71
27	C	520	LHG	C27-C26-C25	-2.12	103.69	114.42
23	7	307	CHL	CED-O2D-CGD	2.12	120.72	115.94
24	d	402	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	N	603	CLA	CHB-C1B-NB	2.11	126.50	124.26
24	0	614	CLA	CHB-C1B-NB	2.11	126.50	124.26
24	A2	610	CLA	CHB-C1B-NB	2.11	126.50	124.26
29	R	410	BCR	C11-C10-C9	-2.11	124.29	127.31
29	v	617	BCR	C7-C8-C9	-2.11	123.04	126.23
23	BB	306	CHL	CED-O2D-CGD	2.11	120.72	115.94
24	A6	612	CLA	CHC-C4B-NB	2.11	126.50	124.26
24	BQ	604	CLA	CHB-C1B-NB	2.11	126.50	124.26
29	Av	101	BCR	C15-C14-C13	-2.11	124.29	127.31
23	N	606	CHL	C4A-NA-C1A	2.11	107.66	106.71
34	1	516	DGD	CBB-CAB-C9B	-2.11	103.70	114.42
23	y	302	CHL	OMC-CMC-C2C	-2.11	120.91	125.69
29	a	411	BCR	C15-C14-C13	-2.11	124.30	127.31
24	y	315	CLA	CHB-C1B-NB	2.11	126.49	124.26
23	8	307	CHL	OMC-CMC-C2C	-2.11	120.91	125.69
24	BG	402	CLA	O2A-CGA-O1A	-2.11	118.26	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	506	CLA	O2D-CGD-CBD	2.11	115.02	111.27
24	y	313	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
31	D	403	PL9	C36-C34-C33	-2.11	116.85	121.12
23	r	613	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
23	r	613	CHL	CMA-C3A-C2A	-2.11	111.17	116.10
23	0	601	CHL	C2A-C1A-CHA	-2.11	120.17	123.86
34	1	518	DGD	O2D-C2D-C1D	-2.11	104.92	110.05
24	G	612	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	C	511	CLA	C1-C2-C3	-2.11	122.39	126.04
24	Y	312	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
27	w	201	LHG	C27-C26-C25	-2.11	103.72	114.42
23	8	306	CHL	CED-O2D-CGD	2.11	120.71	115.94
24	G	604	CLA	CHB-C1B-NB	2.11	126.49	124.26
24	0	603	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	A2	605	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
38	BD	408	PHO	CMB-C2B-C3B	2.11	128.62	124.68
24	BF	511	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	G	602	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
25	BV	615	LUT	C1-C6-C5	-2.11	119.64	122.61
23	7	308	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
24	B	610	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	S	601	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
25	6	615	LUT	C15-C35-C34	2.11	127.79	123.47
23	s	605	CHL	CHC-C4B-NB	-2.11	122.03	124.26
24	B	613	CLA	CHB-C1B-NB	2.11	126.49	124.26
24	BB	315	CLA	CHC-C4B-NB	2.11	126.49	124.26
24	Aw	102	CLA	C2D-C1D-ND	-2.11	108.55	110.10
30	B	620	LMG	O2-C2-C1	-2.11	104.93	110.05
29	z	101	BCR	C16-C15-C14	-2.11	119.16	123.47
28	r	616	XAT	C17-C1-C16	2.11	110.48	107.37
23	Ba	307	CHL	O2A-CGA-O1A	-2.11	118.28	123.59
23	AB	307	CHL	O2A-CGA-CBA	2.11	120.80	114.03
30	A0	201	LMG	O8-C28-O10	-2.11	118.28	123.59
30	v	623	LMG	O3-C3-C2	-2.11	105.48	110.35
24	AA	304	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
23	Au	609	CHL	C6-C5-C3	-2.11	111.18	114.62
32	l	102	SQD	C45-O47-C7	-2.11	112.61	117.79
24	BF	507	CLA	O1D-CGD-CBD	2.10	128.79	124.48
24	Ba	303	CLA	CHB-C1B-NB	2.10	126.48	124.26
27	b	624	LHG	C18-C17-C16	-2.10	103.74	114.42
29	1	514	BCR	C15-C16-C17	-2.10	119.16	123.47
24	n	614	CLA	CED-O2D-CGD	2.10	120.70	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	603	CLA	CMB-C2B-C1B	-2.10	122.16	125.37
24	6	602	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
38	R	407	PHO	C1C-C2C-C3C	-2.10	106.86	108.61
24	n	603	CLA	CHB-C1B-NB	2.10	126.48	124.26
24	r	602	CLA	CHB-C1B-NB	2.10	126.48	124.26
24	BF	504	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	BV	607	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
24	AB	308	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
24	C	508	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
24	9	613	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
23	BQ	609	CHL	C4A-NA-C1A	2.10	107.65	106.71
24	BB	312	CLA	C2D-C1D-ND	-2.10	108.56	110.10
24	Y	315	CLA	O2D-CGD-CBD	2.10	115.00	111.27
30	i	101	LMG	O3-C3-C2	-2.10	105.49	110.35
24	b	613	CLA	C1-C2-C3	-2.10	122.41	126.04
29	BE	620	BCR	C15-C16-C17	-2.10	119.17	123.47
23	AA	307	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
30	BL	101	LMG	O3-C3-C2	-2.10	105.49	110.35
24	Y	311	CLA	C3B-C4B-NB	-2.10	108.57	110.52
24	v	614	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	n	604	CLA	CHC-C4B-NB	2.10	126.48	124.26
34	BD	401	DGD	CAB-C9B-C8B	-2.10	103.76	114.42
24	c	507	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	AA	302	CHL	C4A-NA-C1A	2.10	107.65	106.71
24	BE	613	CLA	C1-C2-C3	-2.10	122.41	126.04
31	2	404	PL9	C36-C34-C33	-2.10	116.87	121.12
23	n	606	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
24	v	608	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
24	c	513	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
24	1	504	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
30	B	624	LMG	O3-C3-C2	-2.10	105.50	110.35
23	9	601	CHL	O2A-CGA-CBA	2.10	120.77	114.03
24	AA	312	CLA	CHD-C1D-ND	-2.10	122.53	124.45
24	1	509	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	Y	307	CHL	CAA-C2A-C1A	2.10	118.85	111.97
24	c	506	CLA	C2D-C1D-ND	-2.10	108.56	110.10
24	1	508	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
23	AA	308	CHL	O2D-CGD-O1D	-2.10	119.74	123.84
24	S	611	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	AA	316	LUT	C15-C35-C34	2.10	127.77	123.47
24	c	507	CLA	C1-C2-C3	-2.10	122.42	126.04
31	d	403	PL9	C37-C38-C39	-2.10	122.61	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	v	619	BCR	C8-C7-C6	-2.10	121.31	127.20
23	7	307	CHL	C4D-CHA-C1A	-2.10	118.70	121.25
24	BE	611	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
24	s	613	CLA	CHC-C4B-NB	2.10	126.47	124.26
25	S	614	LUT	C31-C30-C29	2.10	130.30	127.31
30	I	101	LMG	O1-C7-C8	-2.09	105.84	110.90
29	b	620	BCR	C15-C16-C17	-2.09	119.18	123.47
24	Au	604	CLA	CHB-C1B-NB	2.09	126.47	124.26
34	a	413	DGD	CBB-CAB-C9B	-2.09	103.80	114.42
24	BB	305	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	Ay	102	BCR	C8-C7-C6	-2.09	121.32	127.20
23	0	607	CHL	CHC-C4B-NB	-2.09	122.04	124.26
24	g	602	CLA	CHD-C1D-ND	-2.09	122.53	124.45
30	BF	501	LMG	O2-C2-C1	-2.09	104.96	110.05
24	s	612	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
30	A	412	LMG	O3-C3-C2	-2.09	105.51	110.35
23	AB	306	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
27	9	618	LHG	C27-C26-C25	-2.09	103.81	114.42
23	r	613	CHL	CAA-C2A-C3A	-2.09	111.22	116.10
24	s	603	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	A	407	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	BU	608	CLA	CHB-C1B-NB	2.09	126.47	124.26
23	g	608	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
34	a	401	DGD	CAB-C9B-C8B	-2.09	103.82	114.42
23	g	605	CHL	O2A-CGA-CBA	2.09	120.74	114.03
23	s	607	CHL	CED-O2D-CGD	2.09	120.66	115.94
28	BU	616	XAT	C17-C1-C16	2.09	110.45	107.37
30	Aw	101	LMG	O3-C3-C2	-2.09	105.52	110.35
23	6	601	CHL	C2A-C1A-CHA	-2.09	120.21	123.86
24	C	509	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	Ba	315	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	BU	610	CLA	CHB-C1B-NB	2.09	126.47	124.26
30	v	620	LMG	O2-C2-C1	-2.09	104.97	110.05
23	N	608	CHL	C1C-C2C-C3C	-2.09	105.46	107.11
24	Ba	304	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
27	L	102	LHG	C5-O7-C7	-2.09	112.65	117.79
23	BV	605	CHL	OMC-CMC-C2C	-2.09	120.97	125.69
30	Aw	101	LMG	O1-C1-C2	-2.09	105.05	108.30
24	AA	311	CLA	CHC-C4B-NB	2.09	126.47	124.26
25	BQ	616	LUT	C1-C6-C5	-2.09	119.67	122.61
34	BF	517	DGD	O2D-C2D-C1D	-2.09	104.98	110.05
31	BG	403	PL9	O2-C1-C2	-2.09	117.00	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BJ	602	CLA	CHB-C1B-NB	2.09	126.47	124.26
30	BL	101	LMG	C6-C5-C4	-2.09	108.12	113.00
34	BD	413	DGD	CBB-CAB-C9B	-2.09	103.84	114.42
24	B	614	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
24	A6	611	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	BJ	605	CHL	O2A-CGA-CBA	2.09	120.73	114.03
24	0	611	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
24	BF	504	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
32	2	408	SQD	O5-C5-C4	2.08	113.48	109.69
24	7	311	CLA	CHB-C1B-NB	2.08	126.46	124.26
24	y	312	CLA	CHB-C1B-NB	2.08	126.46	124.26
24	b	615	CLA	CMB-C2B-C1B	-2.08	122.19	125.37
23	9	609	CHL	CHD-C1D-C2D	2.08	129.85	125.48
24	N	610	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
24	n	612	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	N	607	CHL	OMC-CMC-C2C	-2.08	120.97	125.69
23	8	306	CHL	C4D-CHA-C1A	-2.08	118.71	121.25
24	BQ	603	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	s	607	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
29	b	601	BCR	C11-C10-C9	-2.08	124.34	127.31
25	8	311	LUT	C39-C29-C28	2.08	121.36	118.08
24	A	410	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
31	2	404	PL9	O2-C1-C6	2.08	124.20	120.59
24	G	612	CLA	CHB-C1B-NB	2.08	126.46	124.26
23	Y	308	CHL	OMC-CMC-C2C	-2.08	120.98	125.69
24	B	611	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	y	311	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
24	b	613	CLA	CHC-C4B-NB	2.08	126.46	124.26
23	Y	302	CHL	O2A-CGA-O1A	-2.08	118.34	123.59
24	C	504	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	Y	309	CHL	O2A-CGA-CBA	2.08	118.44	111.91
32	d	406	SQD	C45-O47-C7	-2.08	112.67	117.79
24	Au	612	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	8	307	CHL	O2A-CGA-CBA	2.08	120.71	114.03
24	BE	615	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
24	BE	602	CLA	CHB-C1B-NB	2.08	126.46	124.26
29	8	313	BCR	C35-C13-C14	-2.08	120.01	122.92
29	k	101	BCR	C8-C7-C6	-2.08	121.36	127.20
24	d	401	CLA	O2D-CGD-CBD	2.08	114.96	111.27
24	2	402	CLA	C1-C2-C3	-2.08	122.45	126.04
26	AA	319	NEX	C10-C11-C12	2.08	129.71	123.22
23	AA	308	CHL	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	611	CLA	CHB-C1B-NB	2.08	126.46	124.26
24	A6	613	CLA	CHB-C1B-NB	2.08	126.46	124.26
23	BB	307	CHL	CAA-CBA-CGA	-2.08	107.18	113.25
24	b	611	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	BH	601	CHL	O2D-CGD-O1D	-2.08	119.37	124.09
24	C	506	CLA	C2D-C1D-ND	-2.08	108.57	110.10
24	n	612	CLA	C1-C2-C3	-2.08	122.45	126.04
24	S	609	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
24	1	508	CLA	CHB-C1B-NB	2.08	126.46	124.26
38	A	408	PHO	C2D-C1D-ND	-2.08	108.09	109.53
23	BJ	607	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
23	0	608	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
24	n	602	CLA	CHD-C1D-ND	-2.08	122.55	124.45
24	BF	503	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
29	K	102	BCR	C8-C7-C6	-2.07	121.38	127.20
24	6	611	CLA	C1-C2-C3	-2.07	122.45	126.04
31	d	403	PL9	O2-C1-C2	-2.07	117.03	121.78
27	W	201	LHG	C18-C17-C16	-2.07	103.89	114.42
24	B	602	CLA	CHB-C1B-NB	2.07	126.45	124.26
24	y	303	CLA	CHB-C1B-NB	2.07	126.45	124.26
23	6	607	CHL	C2A-C1A-CHA	-2.07	120.23	123.86
26	7	319	NEX	C10-C11-C12	2.07	129.69	123.22
24	7	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45
24	G	611	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	Y	307	CHL	CAA-CBA-CGA	-2.07	107.19	113.25
24	0	610	CLA	CHC-C1C-NC	2.07	127.35	124.20
23	5	601	CHL	O2A-CGA-CBA	2.07	120.69	114.03
25	n	616	LUT	C19-C9-C8	2.07	121.34	118.08
24	A6	609	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	BQ	612	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	BU	603	CLA	CHB-C1B-NB	2.07	126.45	124.26
34	c	516	DGD	O3G-C1D-C2D	-2.07	105.07	108.30
27	BG	404	LHG	C27-C26-C25	-2.07	103.90	114.42
23	BB	310	CHL	CHC-C4B-NB	-2.07	122.06	124.26
24	N	610	CLA	CHB-C1B-NB	2.07	126.45	124.26
24	0	602	CLA	CHC-C4B-NB	2.07	126.45	124.26
24	AA	314	CLA	CHC-C4B-NB	2.07	126.45	124.26
24	g	611	CLA	C1-C2-C3	-2.07	122.46	126.04
24	BF	507	CLA	C1-C2-C3	-2.07	122.46	126.04
25	Y	317	LUT	C19-C9-C8	2.07	121.34	118.08
24	6	611	CLA	C2D-C1D-ND	-2.07	108.58	110.10
34	A	402	DGD	CAB-C9B-C8B	-2.07	103.91	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	614	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	G	601	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
23	g	601	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
24	0	611	CLA	C2D-C1D-ND	-2.07	108.58	110.10
24	c	511	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	s	614	LUT	C31-C30-C29	2.07	130.26	127.31
24	b	611	CLA	CHB-C1B-NB	2.07	126.45	124.26
29	1	514	BCR	C2-C1-C6	2.07	113.67	110.48
23	AA	310	CHL	O2A-CGA-CBA	2.07	118.40	111.91
29	f	101	BCR	C15-C16-C17	-2.07	119.23	123.47
23	BJ	601	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
24	N	614	CLA	O2D-CGD-CBD	2.07	114.94	111.27
24	R	404	CLA	O2D-CGD-CBD	2.07	114.94	111.27
34	h	102	DGD	C3D-C4D-C5D	-2.07	106.55	110.24
25	Y	317	LUT	C39-C29-C28	2.07	121.34	118.08
24	AA	315	CLA	CHB-C1B-NB	2.07	126.45	124.26
24	6	604	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
27	b	622	LHG	C18-C17-C16	-2.07	103.93	114.42
27	BE	622	LHG	C18-C17-C16	-2.07	103.93	114.42
24	Au	610	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
27	w	201	LHG	C18-C17-C16	-2.07	103.93	114.42
23	s	601	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
24	7	304	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	C	504	CLA	C1-C2-C3	-2.07	122.47	126.04
27	A0	202	LHG	C18-C17-C16	-2.07	103.93	114.42
34	R	401	DGD	CAB-C9B-C8B	-2.07	103.93	114.42
24	v	604	CLA	CHC-C4B-NB	2.07	126.44	124.26
24	g	610	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	BQ	612	CLA	C1-C2-C3	-2.07	122.47	126.04
30	BL	101	LMG	O8-C28-O10	-2.07	118.38	123.59
27	0	617	LHG	C18-C17-C16	-2.07	103.94	114.42
24	G	610	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	b	616	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
23	BJ	608	CHL	O1D-CGD-CBD	-2.07	120.26	124.48
24	BV	609	CLA	CHD-C1D-ND	-2.07	122.56	124.45
24	A	407	CLA	C2D-C1D-ND	-2.07	108.58	110.10
34	A	402	DGD	CBB-CAB-C9B	-2.07	103.94	114.42
23	Ba	310	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
24	Au	610	CLA	CHB-C1B-NB	2.06	126.44	124.26
34	BD	413	DGD	O6E-C1E-O5D	-2.06	105.08	109.97
27	v	621	LHG	C18-C17-C16	-2.06	103.94	114.42
23	y	302	CHL	C2A-C1A-CHA	-2.06	120.25	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A0	201	LMG	C6-C5-C4	-2.06	108.17	113.00
24	BQ	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
24	BE	610	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	0	613	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	A6	613	CLA	CHC-C4B-NB	2.06	126.44	124.26
24	5	610	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	6	608	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
23	A2	601	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
23	s	605	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
23	Ba	309	CHL	CAA-C2A-C3A	-2.06	107.13	112.78
24	AB	301	CLA	CAC-C3C-C4C	2.06	127.48	124.81
23	9	609	CHL	C1D-CHD-C4C	-2.06	121.61	126.06
23	7	302	CHL	CHD-C1D-C2D	2.06	129.80	125.48
29	v	619	BCR	C38-C26-C25	-2.06	122.21	124.53
38	R	407	PHO	O2A-CGA-O1A	-2.06	118.39	123.59
24	N	611	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	BJ	610	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	AA	303	CLA	C1-C2-C3	-2.06	122.48	126.04
23	A6	601	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
34	R	401	DGD	CBB-CAB-C9B	-2.06	103.97	114.42
34	BF	517	DGD	C5B-C4B-C3B	-2.06	103.97	114.42
24	b	602	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	Au	613	CLA	CHC-C4B-NB	2.06	126.44	124.26
23	AB	304	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
23	BJ	605	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
23	BU	605	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
23	8	304	CHL	C1D-ND-C4D	-2.06	104.87	106.33
23	e	601	CHL	O2A-CGA-CBA	2.06	120.65	114.03
24	a	410	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
24	1	513	CLA	CAA-C2A-C1A	2.06	118.72	111.97
24	G	603	CLA	CHD-C1D-ND	-2.06	122.56	124.45
24	A2	611	CLA	C2D-C1D-ND	-2.06	108.59	110.10
23	Au	607	CHL	CED-O2D-CGD	2.06	120.59	115.94
23	G	601	CHL	CHC-C4B-NB	-2.06	122.08	124.26
31	BG	403	PL9	C12-C13-C14	-2.06	122.70	127.66
23	7	308	CHL	CBB-CAB-C3B	-2.06	117.38	127.62
24	I	102	CLA	O2D-CGD-CBD	2.06	114.92	111.27
24	0	610	CLA	O2D-CGD-CBD	2.06	114.92	111.27
24	C	508	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	Ba	312	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	v	612	CLA	C2D-C1D-ND	-2.06	108.59	110.10
24	a	410	CLA	CAA-CBA-CGA	-2.06	107.24	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	617	BCR	C35-C13-C14	-2.06	120.04	122.92
24	AB	308	CLA	CMB-C2B-C3B	2.06	131.57	126.59
29	v	618	BCR	C8-C7-C6	-2.06	121.43	127.20
24	c	512	CLA	CHB-C1B-NB	2.06	126.43	124.26
24	N	602	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	2	402	CLA	C2D-C1D-ND	-2.06	108.59	110.10
24	B	605	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
27	6	617	LHG	C18-C17-C16	-2.06	103.99	114.42
24	7	314	CLA	CHC-C4B-NB	2.06	126.43	124.26
24	C	512	CLA	CHB-C1B-NB	2.06	126.43	124.26
24	Au	602	CLA	CHB-C1B-NB	2.06	126.43	124.26
24	BV	613	CLA	CHC-C4B-NB	2.06	126.43	124.26
25	BQ	616	LUT	C11-C10-C9	2.06	130.24	127.31
23	AA	306	CHL	C4D-CHA-C1A	-2.06	118.75	121.25
23	g	607	CHL	O2D-CGD-O1D	-2.05	119.82	123.84
23	n	606	CHL	O2D-CGD-O1D	-2.05	119.82	123.84
24	6	603	CLA	CHB-C1B-NB	2.05	126.43	124.26
24	Y	304	CLA	CHB-C1B-NB	2.05	126.43	124.26
23	0	609	CHL	O2A-CGA-CBA	2.05	118.35	111.91
24	1	505	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
24	A6	612	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
28	r	616	XAT	C4-C3-C2	-2.05	106.81	110.77
24	S	613	CLA	CHB-C1B-NB	2.05	126.43	124.26
29	B	617	BCR	C7-C8-C9	-2.05	123.13	126.23
24	a	405	CLA	CHC-C4B-NB	2.05	126.43	124.26
24	Aw	102	CLA	CHC-C4B-NB	2.05	126.43	124.26
29	Bb	101	BCR	C35-C13-C14	-2.05	120.05	122.92
23	r	606	CHL	C1D-CHD-C4C	-2.05	121.63	126.06
29	B	618	BCR	C8-C7-C6	-2.05	121.44	127.20
24	BB	311	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
27	r	618	LHG	C27-C26-C25	-2.05	104.01	114.42
24	Au	611	CLA	C2D-C1D-ND	-2.05	108.59	110.10
24	B	601	CLA	C1-C2-C3	-2.05	122.50	126.04
29	BF	515	BCR	C16-C15-C14	-2.05	119.27	123.47
24	6	611	CLA	CHC-C4B-NB	2.05	126.43	124.26
24	G	613	CLA	CHC-C4B-NB	2.05	126.43	124.26
24	Aw	102	CLA	O2D-CGD-CBD	2.05	114.91	111.27
24	Ba	313	CLA	C2D-C1D-ND	-2.05	108.59	110.10
23	G	601	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
27	B	621	LHG	C18-C17-C16	-2.05	104.02	114.42
23	AB	304	CHL	O2A-CGA-CBA	2.05	120.61	114.03
34	c	516	DGD	C5B-C4B-C3B	-2.05	104.02	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	612	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
29	K	101	BCR	C15-C16-C17	-2.05	119.28	123.47
24	v	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	c	509	CLA	C1-C2-C3	-2.05	122.50	126.04
24	n	614	CLA	CHD-C1D-ND	-2.05	122.57	124.45
24	c	504	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	BB	309	CHL	O2A-CGA-CBA	2.05	118.33	111.91
23	6	601	CHL	CHB-C4A-NA	2.05	127.34	124.51
23	Ba	302	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
24	A2	603	CLA	CHB-C1B-NB	2.05	126.42	124.26
24	BV	610	CLA	CHB-C1B-NB	2.05	126.42	124.26
24	BF	509	CLA	CHB-C1B-NB	2.05	126.42	124.26
24	B	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	C	509	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	r	612	CLA	C2D-C1D-ND	-2.05	108.59	110.10
29	v	617	BCR	C35-C13-C14	-2.05	120.06	122.92
24	n	612	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
24	BF	503	CLA	CHB-C1B-NB	2.05	126.42	124.26
23	Au	607	CHL	O2A-CGA-O1A	-2.05	118.43	123.59
27	BE	624	LHG	C5-O7-C7	-2.05	112.75	117.79
23	A2	606	CHL	CAA-CBA-CGA	-2.05	107.27	113.25
24	BE	612	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
24	y	304	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	0	602	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	r	606	CHL	C4A-NA-C1A	2.05	107.63	106.71
34	1	516	DGD	O2D-C2D-C1D	-2.05	105.08	110.05
24	BD	407	CLA	C2D-C1D-ND	-2.05	108.60	110.10
30	1	501	LMG	C1-O6-C5	-2.05	109.67	113.69
24	0	604	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
24	b	610	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	BJ	607	CHL	CHB-C1B-C2B	-2.05	121.46	127.24
23	AA	308	CHL	CBB-CAB-C3B	-2.05	117.44	127.62
29	H	101	BCR	C2-C1-C6	2.05	113.63	110.48
29	BI	101	BCR	C15-C16-C17	-2.05	119.28	123.47
24	BQ	602	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	BF	509	CLA	C1-C2-C3	-2.05	122.51	126.04
23	7	306	CHL	O2A-CGA-CBA	2.04	120.60	114.03
24	S	613	CLA	C2D-C1D-ND	-2.04	108.60	110.10
24	r	612	CLA	CHD-C1D-ND	-2.04	122.58	124.45
27	d	404	LHG	C27-C26-C25	-2.04	104.05	114.42
24	Y	304	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	0	615	LUT	C39-C29-C28	2.04	121.30	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BE	612	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	A6	615	LUT	C11-C10-C9	2.04	130.23	127.31
23	g	607	CHL	CHB-C1B-C2B	-2.04	121.47	127.24
24	BJ	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
38	A	408	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
34	a	413	DGD	O6E-C1E-O5D	-2.04	105.14	109.97
24	BB	305	CLA	CHB-C1B-NB	2.04	126.42	124.26
23	7	310	CHL	O2A-CGA-CBA	2.04	118.32	111.91
30	A0	201	LMG	O3-C3-C2	-2.04	105.63	110.35
23	5	601	CHL	C1C-C2C-C3C	-2.04	105.49	107.11
23	AA	310	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
23	7	306	CHL	C4D-CHA-C1A	-2.04	118.76	121.25
24	BF	508	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	1	502	CLA	C2D-C1D-ND	-2.04	108.60	110.10
24	0	611	CLA	CHB-C1B-NB	2.04	126.42	124.26
23	6	606	CHL	C4D-CHA-C1A	-2.04	118.76	121.25
25	BB	317	LUT	C35-C34-C33	2.04	130.22	127.31
24	7	311	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	d	401	CLA	C1-C2-C3	-2.04	122.51	126.04
24	0	614	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	v	608	CLA	CHC-C4B-NB	2.04	126.42	124.26
34	Av	102	DGD	C3D-C4D-C5D	-2.04	106.60	110.24
24	BQ	603	CLA	C1-C2-C3	-2.04	122.51	126.04
24	C	505	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	5	611	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
23	AA	306	CHL	O2A-CGA-CBA	2.04	120.59	114.03
23	0	605	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
24	7	315	CLA	CHB-C1B-NB	2.04	126.42	124.26
24	G	610	CLA	CHB-C1B-NB	2.04	126.42	124.26
24	BV	603	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	s	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	AA	316	LUT	C7-C8-C9	-2.04	123.15	126.23
24	0	611	CLA	CHC-C4B-NB	2.04	126.42	124.26
24	1	506	CLA	CHB-C1B-NB	2.04	126.42	124.26
24	AA	313	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
29	BF	516	BCR	C24-C23-C22	-2.04	123.16	126.23
23	7	302	CHL	C1D-ND-C4D	-2.04	104.89	106.33
24	BJ	613	CLA	CHD-C1D-ND	-2.04	122.58	124.45
27	BU	617	LHG	C27-C26-C25	-2.04	104.08	114.42
24	BB	304	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	6	615	LUT	C7-C8-C9	-2.04	123.16	126.23
25	S	615	LUT	C7-C8-C9	2.04	129.31	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BJ	611	CLA	C1-C2-C3	-2.04	122.52	126.04
24	B	615	CLA	CHB-C1B-NB	2.04	126.41	124.26
24	b	606	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	9	610	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
27	b	624	LHG	C5-O7-C7	-2.04	112.78	117.79
24	9	602	CLA	C2D-C1D-ND	-2.04	108.60	110.10
23	BJ	606	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
24	R	406	CLA	CHB-C1B-NB	2.04	126.41	124.26
24	BV	612	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
24	BE	606	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	R	409	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
27	BY	201	LHG	C18-C17-C16	-2.04	104.09	114.42
24	8	308	CLA	O1A-CGA-CBA	2.04	129.62	123.08
24	a	410	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	A2	607	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
23	y	309	CHL	CAA-C2A-C3A	-2.04	107.20	112.78
24	s	609	CLA	CHD-C1D-ND	-2.03	122.58	124.45
24	n	613	CLA	CAC-C3C-C4C	2.03	127.45	124.81
24	n	603	CLA	C1-C2-C3	-2.03	122.52	126.04
24	8	309	CLA	CHB-C1B-NB	2.03	126.41	124.26
24	A6	613	CLA	O1D-CGD-CBD	2.03	128.65	124.48
30	c	518	LMG	O3-C3-C2	-2.03	105.65	110.35
24	1	509	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	Y	312	CLA	C2D-C1D-ND	-2.03	108.61	110.10
24	A2	614	CLA	O2D-CGD-CBD	2.03	114.88	111.27
25	g	616	LUT	C12-C13-C14	2.03	122.06	118.94
24	A2	611	CLA	CHB-C1B-NB	2.03	126.41	124.26
23	6	609	CHL	CHC-C1C-NC	-2.03	121.12	124.20
24	BV	602	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	S	615	LUT	C7-C6-C5	-2.03	116.54	121.46
24	5	603	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	BV	613	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	BU	609	CLA	CHB-C1B-NB	2.03	126.41	124.26
23	BQ	608	CHL	CAA-C2A-C1A	2.03	118.63	111.97
25	G	616	LUT	C39-C29-C28	2.03	121.28	118.08
34	C	516	DGD	C5B-C4B-C3B	-2.03	104.11	114.42
23	n	601	CHL	C2A-C1A-CHA	-2.03	120.31	123.86
25	A2	616	LUT	C8-C9-C10	2.03	122.06	118.94
23	5	605	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
23	Au	607	CHL	OMC-CMC-C2C	-2.03	121.09	125.69
34	a	413	DGD	O2D-C2D-C1D	-2.03	105.11	110.05
38	a	409	PHO	O2A-CGA-O1A	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	S	607	CHL	CED-O2D-CGD	2.03	120.53	115.94
24	AB	308	CLA	CAC-C3C-C4C	2.03	127.44	124.81
24	BJ	604	CLA	CHB-C1B-NB	2.03	126.41	124.26
24	N	611	CLA	C1-C2-C3	-2.03	122.53	126.04
23	AB	306	CHL	CED-O2D-CGD	2.03	120.53	115.94
23	g	605	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
24	c	507	CLA	O1D-CGD-CBD	2.03	128.63	124.48
24	1	513	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
30	i	101	LMG	O8-C28-O10	-2.03	118.47	123.59
24	S	602	CLA	C2D-C1D-ND	-2.03	108.61	110.10
31	d	403	PL9	O2-C1-C6	2.03	124.10	120.59
29	BK	101	BCR	C8-C7-C6	-2.03	121.50	127.20
24	BB	303	CLA	C1-C2-C3	-2.03	122.53	126.04
24	n	602	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	C	506	CLA	CHB-C1B-NB	2.03	126.40	124.26
25	s	614	LUT	C32-C33-C34	2.03	122.05	118.94
29	b	618	BCR	C7-C8-C9	-2.03	123.17	126.23
38	BD	409	PHO	C2D-C1D-ND	-2.03	108.13	109.53
34	a	401	DGD	O5D-C6D-C5D	-2.03	105.30	109.05
24	BE	616	CLA	O2D-CGD-CBD	2.03	114.87	111.27
24	BQ	612	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
24	r	610	CLA	C2D-C1D-ND	-2.03	108.61	110.10
24	v	610	CLA	C2D-C1D-ND	-2.03	108.61	110.10
24	9	603	CLA	C1-C2-C3	-2.03	122.54	126.04
24	Y	315	CLA	CHC-C4B-NB	2.03	126.40	124.26
24	AB	309	CLA	CHB-C1B-NB	2.03	126.40	124.26
34	C	518	DGD	O3E-C3E-C2E	-2.03	105.66	110.35
23	BU	605	CHL	C1D-CHD-C4C	-2.03	121.69	126.06
23	A2	606	CHL	C4A-NA-C1A	2.03	107.62	106.71
33	4	102	HEM	C2A-C1A-NA	-2.03	107.88	110.15
24	c	502	CLA	C2D-C1D-ND	-2.03	108.61	110.10
24	AA	303	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
23	BH	601	CHL	O2A-CGA-CBA	2.03	120.54	114.03
31	BG	403	PL9	O2-C1-C6	2.03	124.10	120.59
23	0	607	CHL	OMC-CMC-C2C	-2.03	121.11	125.69
23	Au	609	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
30	BE	621	LMG	O7-C10-O9	-2.03	118.81	123.70
24	9	603	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
29	Ay	101	BCR	C15-C14-C13	-2.02	124.42	127.31
23	S	607	CHL	C4D-CHA-C1A	-2.02	118.78	121.25
27	5	618	LHG	C27-C26-C25	-2.02	104.15	114.42
29	A	411	BCR	C15-C16-C17	-2.02	119.33	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	311	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
24	v	602	CLA	CHB-C1B-NB	2.02	126.40	124.26
24	BQ	604	CLA	CHC-C4B-NB	2.02	126.40	124.26
23	8	306	CHL	OMC-CMC-C2C	-2.02	121.11	125.69
23	5	606	CHL	O1D-CGD-CBD	-2.02	120.34	124.48
24	9	611	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
24	BD	410	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
24	0	603	CLA	CHB-C1B-NB	2.02	126.40	124.26
24	BU	612	CLA	C2D-C1D-ND	-2.02	108.61	110.10
24	0	614	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	BE	602	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
34	1	516	DGD	O3E-C3E-C2E	-2.02	105.67	110.35
24	BF	504	CLA	C1-C2-C3	-2.02	122.55	126.04
34	c	516	DGD	C1D-C2D-C3D	-2.02	105.78	110.00
23	n	608	CHL	CAA-C2A-C1A	2.02	118.60	111.97
23	y	308	CHL	CBB-CAB-C3B	-2.02	117.56	127.62
24	0	604	CLA	CHD-C1D-ND	-2.02	122.60	124.45
34	C	516	DGD	O3E-C3E-C2E	-2.02	105.67	110.35
34	1	516	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
24	c	503	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	BD	410	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	r	604	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
29	AB	313	BCR	C15-C16-C17	-2.02	119.33	123.47
23	G	607	CHL	CED-O2D-CGD	2.02	120.51	115.94
34	1	518	DGD	C5B-C4B-C3B	-2.02	104.17	114.42
24	b	617	CLA	CHB-C1B-NB	2.02	126.40	124.26
31	BG	403	PL9	C32-C33-C34	-2.02	122.80	127.66
24	s	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	D	401	CLA	C1-C2-C3	-2.02	122.55	126.04
24	A2	602	CLA	CHD-C1D-ND	-2.02	122.60	124.45
24	s	610	CLA	CHB-C1B-NB	2.02	126.39	124.26
23	Au	605	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
23	0	605	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
24	BG	401	CLA	C2D-C1D-ND	-2.02	108.62	110.10
24	R	405	CLA	CHD-C1D-C2D	2.02	129.72	125.48
24	N	610	CLA	CMB-C2B-C3B	2.02	131.48	126.59
24	S	613	CLA	O1D-CGD-CBD	2.02	128.62	124.48
23	N	607	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
30	c	518	LMG	O1-C7-C8	-2.02	106.03	110.90
24	BF	509	CLA	CHC-C4B-NB	2.02	126.39	124.26
24	AA	313	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
23	9	606	CHL	O1D-CGD-CBD	-2.02	120.35	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BU	607	CHL	OMC-CMC-C2C	-2.02	121.12	125.69
24	v	605	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	A2	615	LUT	C31-C30-C29	2.02	130.19	127.31
24	0	611	CLA	C1-C2-C3	-2.02	122.55	126.04
34	C	517	DGD	C5B-C4B-C3B	-2.02	104.18	114.42
24	v	603	CLA	C2D-C1D-ND	-2.02	108.62	110.10
23	5	601	CHL	CHC-C4B-NB	-2.02	122.12	124.26
34	a	413	DGD	C3D-C4D-C5D	-2.02	106.64	110.24
34	1	518	DGD	O3E-C3E-C2E	-2.02	105.69	110.35
23	9	606	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
23	BU	605	CHL	C3C-C4C-NC	2.02	112.83	110.57
24	g	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
24	S	612	CLA	C1-C2-C3	-2.02	122.56	126.04
24	S	613	CLA	CHC-C4B-NB	2.02	126.39	124.26
24	0	603	CLA	CHC-C4B-NB	2.02	126.39	124.26
23	Ba	308	CHL	CBB-CAB-C3B	-2.02	117.59	127.62
34	1	517	DGD	C5B-C4B-C3B	-2.02	104.19	114.42
24	R	405	CLA	C2D-C1D-ND	-2.02	108.62	110.10
23	G	601	CHL	C6-C5-C3	-2.02	111.32	114.62
34	h	102	DGD	C1D-C2D-C3D	-2.02	105.80	110.00
29	B	619	BCR	C38-C26-C25	-2.02	122.26	124.53
23	6	605	CHL	CED-O2D-CGD	2.02	120.50	115.94
24	6	611	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	B	608	CLA	CHC-C4B-NB	2.02	126.39	124.26
24	v	615	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	BE	609	CLA	CMB-C2B-C3B	2.02	131.47	126.59
23	Au	606	CHL	CAA-CBA-CGA	-2.02	107.36	113.25
24	y	303	CLA	CHD-C1D-ND	-2.02	122.60	124.45
34	Av	102	DGD	C5B-C4B-C3B	-2.02	104.19	114.42
24	1	506	CLA	C2D-C1D-ND	-2.02	108.62	110.10
24	v	606	CLA	C1-C2-C3	-2.02	122.56	126.04
25	BQ	616	LUT	C32-C33-C34	2.01	122.03	118.94
30	C	501	LMG	C1-O6-C5	-2.01	109.73	113.69
24	7	311	CLA	CHC-C4B-NB	2.01	126.39	124.26
24	BQ	603	CLA	CHB-C1B-NB	2.01	126.39	124.26
23	Ba	308	CHL	CED-O2D-CGD	2.01	120.49	115.94
30	BF	501	LMG	O7-C10-O9	-2.01	118.83	123.70
24	G	603	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	Ba	311	CLA	C1-C2-C3	-2.01	122.56	126.04
29	b	601	BCR	C33-C5-C6	-2.01	122.27	124.53
25	8	311	LUT	C32-C33-C34	2.01	122.03	118.94
23	n	606	CHL	OMC-CMC-C2C	-2.01	121.13	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BB	314	CLA	C2D-C1D-ND	-2.01	108.62	110.10
23	r	607	CHL	OMC-CMC-C2C	-2.01	121.13	125.69
31	BG	403	PL9	C31-C32-C33	-2.01	105.26	111.88
24	b	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	b	612	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
24	8	301	CLA	CAC-C3C-C4C	2.01	127.42	124.81
23	A2	608	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
23	G	605	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
23	BQ	601	CHL	C2A-C1A-CHA	-2.01	120.34	123.86
30	C	519	LMG	O1-C7-C8	-2.01	106.04	110.90
23	N	606	CHL	CAA-CBA-CGA	-2.01	107.37	113.25
34	c	517	DGD	C5B-C4B-C3B	-2.01	104.21	114.42
24	7	303	CLA	C1-C2-C3	-2.01	122.56	126.04
24	C	513	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	Ba	303	CLA	CHD-C1D-ND	-2.01	122.61	124.45
24	n	604	CLA	CHB-C1B-NB	2.01	126.39	124.26
23	Ba	302	CHL	CHB-C4A-NA	2.01	127.29	124.51
34	BK	102	DGD	C5B-C4B-C3B	-2.01	104.21	114.42
23	y	310	CHL	C3B-C4B-NB	2.01	112.38	110.52
23	BQ	606	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
24	Y	305	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	BE	619	BCR	C24-C23-C22	-2.01	123.20	126.23
34	C	516	DGD	C1D-C2D-C3D	-2.01	105.81	110.00
24	g	604	CLA	CHB-C1B-NB	2.01	126.39	124.26
24	BF	505	CLA	CHB-C1B-NB	2.01	126.39	124.26
24	6	611	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	0	605	CHL	CED-O2D-CGD	2.01	120.48	115.94
24	v	601	CLA	C1-C2-C3	-2.01	122.57	126.04
24	Ba	311	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
24	BU	604	CLA	C2D-C1D-ND	-2.01	108.62	110.10
24	BU	610	CLA	C2D-C1D-ND	-2.01	108.62	110.10
34	A	402	DGD	O3E-C3E-C2E	-2.01	105.70	110.35
25	y	316	LUT	C19-C9-C8	2.01	121.24	118.08
25	A6	615	LUT	C7-C6-C5	-2.01	116.59	121.46
24	7	304	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	g	602	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	n	610	CLA	CMB-C2B-C3B	2.01	131.45	126.59
38	BD	409	PHO	O2A-CGA-O1A	-2.01	118.52	123.59
24	BE	608	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
24	N	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
24	s	602	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	G	611	CLA	O2A-CGA-O1A	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	607	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
24	v	614	CLA	O2D-CGD-CBD	2.01	114.84	111.27
24	b	603	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
24	BB	314	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	0	606	CHL	C4D-CHA-C1A	-2.01	118.81	121.25
23	AA	302	CHL	O2A-CGA-CBA	2.01	120.48	114.03
24	N	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	5	606	CHL	O2A-CGA-CBA	2.01	120.47	114.03
29	b	619	BCR	C24-C23-C22	-2.01	123.20	126.23
24	v	601	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	6	612	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
24	Y	315	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
26	N	617	NEX	C28-C29-C30	2.01	122.02	118.94
23	Au	605	CHL	O2A-CGA-CBA	2.01	120.47	114.03
23	S	601	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
23	BU	607	CHL	C2A-C1A-CHA	-2.01	120.35	123.86
24	9	603	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
24	G	603	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
23	y	306	CHL	OMC-CMC-C2C	-2.00	121.15	125.69
33	F	102	HEM	C2A-C1A-NA	-2.00	107.91	110.15
24	1	512	CLA	O2D-CGD-CBD	2.00	114.83	111.27
24	BF	506	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	g	613	CLA	CHD-C1D-ND	-2.00	122.61	124.45
34	C	518	DGD	C5B-C4B-C3B	-2.00	104.25	114.42
23	BB	306	CHL	C4A-NA-C1A	2.00	107.61	106.71
24	A6	608	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
23	BB	302	CHL	C4-C3-C2	-2.00	118.54	123.68
25	5	616	LUT	C11-C12-C13	2.00	132.04	126.42
24	b	608	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
34	BD	413	DGD	O2D-C2D-C1D	-2.00	105.18	110.05
24	v	604	CLA	CHB-C1B-NB	2.00	126.38	124.26
23	8	307	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
23	r	607	CHL	C2A-C1A-CHA	-2.00	120.36	123.86
24	AB	309	CLA	O1D-CGD-CBD	2.00	128.58	124.48
30	A	412	LMG	C6-C5-C4	-2.00	108.31	113.00
23	s	605	CHL	CBA-CAA-C2A	-2.00	107.95	113.86
31	2	404	PL9	C31-C32-C33	-2.00	105.30	111.88
23	BV	605	CHL	CHB-C4A-NA	2.00	127.28	124.51
30	i	101	LMG	C6-C5-C4	-2.00	108.31	113.00
24	BQ	613	CLA	CAC-C3C-C4C	2.00	127.41	124.81
23	A6	601	CHL	C2A-C1A-CHA	-2.00	120.36	123.86
23	AB	307	CHL	CAA-CBA-CGA	-2.00	107.19	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	409	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
24	B	601	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	BB	314	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	B	610	CLA	C2D-C1D-ND	-2.00	108.63	110.10
26	A2	617	NEX	C28-C29-C30	2.00	122.01	118.94
24	b	612	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	BJ	606	CHL	CED-O2D-CGD	2.00	120.46	115.94
24	6	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
24	b	612	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	9	605	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
24	1	509	CLA	C11-C12-C13	-2.00	109.45	115.92
24	c	509	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	AB	310	CLA	CHC-C4B-NB	2.00	126.38	124.26
24	BJ	611	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	BV	613	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	0	603	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
30	BF	519	LMG	O3-C3-C2	-2.00	105.72	110.35
23	9	606	CHL	O2A-CGA-CBA	2.00	120.46	114.03
34	R	401	DGD	O3E-C3E-C2E	-2.00	105.72	110.35

There are no chirality outliers.

All (8915) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	5	601	CHL	C1A-C2A-CAA-CBA
23	5	601	CHL	C3A-C2A-CAA-CBA
23	5	601	CHL	CBD-CGD-O2D-CED
23	5	605	CHL	C1A-C2A-CAA-CBA
23	5	606	CHL	C2B-C3B-CAB-CBB
23	5	606	CHL	C4B-C3B-CAB-CBB
23	5	607	CHL	C3A-C2A-CAA-CBA
23	5	607	CHL	CHA-CBD-CGD-O1D
23	5	607	CHL	CHA-CBD-CGD-O2D
23	5	607	CHL	CAD-CBD-CGD-O1D
23	5	608	CHL	C3A-C2A-CAA-CBA
23	5	608	CHL	C2A-CAA-CBA-CGA
23	5	608	CHL	C1C-C2C-CMC-OMC
23	5	608	CHL	C3C-C2C-CMC-OMC
23	5	608	CHL	CBD-CGD-O2D-CED
23	5	609	CHL	C2A-CAA-CBA-CGA
23	5	609	CHL	C12-C13-C15-C16
23	6	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	6	601	CHL	C4-C3-C5-C6
23	6	601	CHL	C14-C13-C15-C16
23	6	606	CHL	C1A-C2A-CAA-CBA
23	6	606	CHL	C3A-C2A-CAA-CBA
23	6	607	CHL	C3A-C2A-CAA-CBA
23	6	608	CHL	CHA-CBD-CGD-O1D
23	6	608	CHL	CHA-CBD-CGD-O2D
23	7	306	CHL	CBD-CGD-O2D-CED
23	7	307	CHL	CBD-CGD-O2D-CED
23	7	308	CHL	C1A-C2A-CAA-CBA
23	7	308	CHL	C3A-C2A-CAA-CBA
23	7	308	CHL	CBD-CGD-O2D-CED
23	7	308	CHL	C3-C5-C6-C7
23	7	309	CHL	C1A-C2A-CAA-CBA
23	7	309	CHL	C3A-C2A-CAA-CBA
23	7	309	CHL	C1C-C2C-CMC-OMC
23	7	309	CHL	C3C-C2C-CMC-OMC
23	7	310	CHL	C3C-C2C-CMC-OMC
23	8	304	CHL	C1A-C2A-CAA-CBA
23	8	304	CHL	C3A-C2A-CAA-CBA
23	8	304	CHL	C2A-CAA-CBA-CGA
23	8	304	CHL	C1C-C2C-CMC-OMC
23	8	304	CHL	C3C-C2C-CMC-OMC
23	8	305	CHL	CBD-CGD-O2D-CED
23	8	306	CHL	C1A-C2A-CAA-CBA
23	8	306	CHL	C3A-C2A-CAA-CBA
23	8	307	CHL	CBD-CGD-O2D-CED
23	G	601	CHL	C2-C3-C5-C6
23	G	601	CHL	C4-C3-C5-C6
23	G	605	CHL	C3A-C2A-CAA-CBA
23	G	606	CHL	C2B-C3B-CAB-CBB
23	G	606	CHL	C4B-C3B-CAB-CBB
23	G	607	CHL	C1A-C2A-CAA-CBA
23	G	607	CHL	C3A-C2A-CAA-CBA
23	G	608	CHL	C1A-C2A-CAA-CBA
23	G	608	CHL	C3A-C2A-CAA-CBA
23	G	608	CHL	C3C-C2C-CMC-OMC
23	G	608	CHL	C14-C13-C15-C16
23	N	601	CHL	C1A-C2A-CAA-CBA
23	N	601	CHL	C3C-C2C-CMC-OMC
23	N	605	CHL	C1A-C2A-CAA-CBA
23	N	605	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	N	606	CHL	C2B-C3B-CAB-CBB
23	N	606	CHL	C4B-C3B-CAB-CBB
23	N	606	CHL	C1C-C2C-CMC-OMC
23	N	606	CHL	C3C-C2C-CMC-OMC
23	N	606	CHL	CBD-CGD-O2D-CED
23	N	607	CHL	C1A-C2A-CAA-CBA
23	N	607	CHL	C3A-C2A-CAA-CBA
23	N	608	CHL	C1A-C2A-CAA-CBA
23	N	608	CHL	C3C-C2C-CMC-OMC
23	N	608	CHL	CBD-CGD-O2D-CED
23	S	601	CHL	C1C-C2C-CMC-OMC
23	S	601	CHL	C3C-C2C-CMC-OMC
23	S	605	CHL	C1C-C2C-CMC-OMC
23	S	605	CHL	C3C-C2C-CMC-OMC
23	S	606	CHL	CHA-CBD-CGD-O1D
23	S	606	CHL	CHA-CBD-CGD-O2D
23	S	607	CHL	C1A-C2A-CAA-CBA
23	S	607	CHL	C3A-C2A-CAA-CBA
23	S	607	CHL	C1C-C2C-CMC-OMC
23	S	607	CHL	C3C-C2C-CMC-OMC
23	Y	302	CHL	C2-C3-C5-C6
23	Y	302	CHL	C4-C3-C5-C6
23	Y	306	CHL	C1A-C2A-CAA-CBA
23	Y	306	CHL	C3A-C2A-CAA-CBA
23	Y	307	CHL	C1A-C2A-CAA-CBA
23	Y	307	CHL	C3A-C2A-CAA-CBA
23	Y	307	CHL	C1C-C2C-CMC-OMC
23	Y	307	CHL	C3C-C2C-CMC-OMC
23	Y	307	CHL	CBD-CGD-O2D-CED
23	Y	308	CHL	C1A-C2A-CAA-CBA
23	Y	309	CHL	C1C-C2C-CMC-OMC
23	Y	309	CHL	C3C-C2C-CMC-OMC
23	Y	309	CHL	CBD-CGD-O2D-CED
23	Y	310	CHL	CHA-CBD-CGD-O1D
23	Y	310	CHL	CAD-CBD-CGD-O1D
23	Y	310	CHL	CAD-CBD-CGD-O2D
23	Y	310	CHL	C14-C13-C15-C16
23	g	601	CHL	C2-C3-C5-C6
23	g	601	CHL	C4-C3-C5-C6
23	g	605	CHL	CHA-CBD-CGD-O1D
23	g	605	CHL	CHA-CBD-CGD-O2D
23	g	605	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	g	606	CHL	C2B-C3B-CAB-CBB
23	g	606	CHL	C4B-C3B-CAB-CBB
23	g	607	CHL	C1A-C2A-CAA-CBA
23	g	608	CHL	C1A-C2A-CAA-CBA
23	g	608	CHL	C3A-C2A-CAA-CBA
23	g	608	CHL	C1C-C2C-CMC-OMC
23	g	608	CHL	C3C-C2C-CMC-OMC
23	n	601	CHL	CBD-CGD-O2D-CED
23	n	601	CHL	C4-C3-C5-C6
23	n	605	CHL	C1A-C2A-CAA-CBA
23	n	605	CHL	C3A-C2A-CAA-CBA
23	n	606	CHL	C2B-C3B-CAB-CBB
23	n	606	CHL	C4B-C3B-CAB-CBB
23	n	606	CHL	C1C-C2C-CMC-OMC
23	n	606	CHL	C3C-C2C-CMC-OMC
23	n	606	CHL	CBD-CGD-O2D-CED
23	n	607	CHL	C1A-C2A-CAA-CBA
23	n	607	CHL	C3A-C2A-CAA-CBA
23	n	608	CHL	C1A-C2A-CAA-CBA
23	n	608	CHL	C3C-C2C-CMC-OMC
23	n	608	CHL	CBD-CGD-O2D-CED
23	n	609	CHL	C3C-C2C-CMC-OMC
23	s	601	CHL	C1C-C2C-CMC-OMC
23	s	601	CHL	C3C-C2C-CMC-OMC
23	s	605	CHL	C1C-C2C-CMC-OMC
23	s	605	CHL	C3C-C2C-CMC-OMC
23	s	605	CHL	CHA-CBD-CGD-O1D
23	s	605	CHL	CHA-CBD-CGD-O2D
23	s	605	CHL	CAD-CBD-CGD-O1D
23	s	606	CHL	CHA-CBD-CGD-O1D
23	s	606	CHL	CHA-CBD-CGD-O2D
23	s	607	CHL	C1A-C2A-CAA-CBA
23	s	607	CHL	C3A-C2A-CAA-CBA
23	y	306	CHL	C1A-C2A-CAA-CBA
23	y	306	CHL	C3A-C2A-CAA-CBA
23	y	307	CHL	C1C-C2C-CMC-OMC
23	y	307	CHL	C3C-C2C-CMC-OMC
23	y	307	CHL	CBD-CGD-O2D-CED
23	y	308	CHL	C1A-C2A-CAA-CBA
23	y	308	CHL	C3A-C2A-CAA-CBA
23	y	309	CHL	C3C-C2C-CMC-OMC
23	y	309	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	y	310	CHL	C3C-C2C-CMC-OMC
23	y	310	CHL	CAD-CBD-CGD-O1D
23	y	310	CHL	CBD-CGD-O2D-CED
23	r	605	CHL	C1A-C2A-CAA-CBA
23	r	605	CHL	C3A-C2A-CAA-CBA
23	r	605	CHL	C1C-C2C-CMC-OMC
23	r	605	CHL	C3C-C2C-CMC-OMC
23	r	605	CHL	C3-C5-C6-C7
23	r	606	CHL	C3C-C2C-CMC-OMC
23	r	607	CHL	C1A-C2A-CAA-CBA
23	r	607	CHL	C3A-C2A-CAA-CBA
23	r	607	CHL	CHA-CBD-CGD-O1D
23	r	607	CHL	CHA-CBD-CGD-O2D
23	r	607	CHL	CAD-CBD-CGD-O1D
23	9	601	CHL	C1A-C2A-CAA-CBA
23	9	601	CHL	C3A-C2A-CAA-CBA
23	9	601	CHL	CBD-CGD-O2D-CED
23	9	605	CHL	C1A-C2A-CAA-CBA
23	9	606	CHL	C2B-C3B-CAB-CBB
23	9	606	CHL	C4B-C3B-CAB-CBB
23	9	606	CHL	C3C-C2C-CMC-OMC
23	9	607	CHL	C3A-C2A-CAA-CBA
23	9	607	CHL	CHA-CBD-CGD-O1D
23	9	607	CHL	CHA-CBD-CGD-O2D
23	9	608	CHL	C3A-C2A-CAA-CBA
23	9	608	CHL	C1C-C2C-CMC-OMC
23	9	608	CHL	C3C-C2C-CMC-OMC
23	9	608	CHL	CBD-CGD-O2D-CED
23	9	609	CHL	C2A-CAA-CBA-CGA
23	0	601	CHL	C4-C3-C5-C6
23	0	606	CHL	C1A-C2A-CAA-CBA
23	0	606	CHL	C3A-C2A-CAA-CBA
23	0	607	CHL	C3A-C2A-CAA-CBA
23	0	608	CHL	C3C-C2C-CMC-OMC
23	0	608	CHL	CHA-CBD-CGD-O1D
23	0	608	CHL	CHA-CBD-CGD-O2D
23	AA	306	CHL	CBD-CGD-O2D-CED
23	AA	307	CHL	CBD-CGD-O2D-CED
23	AA	308	CHL	C1A-C2A-CAA-CBA
23	AA	308	CHL	C3A-C2A-CAA-CBA
23	AA	308	CHL	CBD-CGD-O2D-CED
23	AA	308	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	AA	309	CHL	C1A-C2A-CAA-CBA
23	AA	309	CHL	C3A-C2A-CAA-CBA
23	AA	309	CHL	C1C-C2C-CMC-OMC
23	AA	309	CHL	C3C-C2C-CMC-OMC
23	AB	304	CHL	C1A-C2A-CAA-CBA
23	AB	304	CHL	C3A-C2A-CAA-CBA
23	AB	304	CHL	C2A-CAA-CBA-CGA
23	AB	304	CHL	C3C-C2C-CMC-OMC
23	AB	305	CHL	C1A-C2A-CAA-CBA
23	AB	305	CHL	CBD-CGD-O2D-CED
23	AB	306	CHL	C1A-C2A-CAA-CBA
23	AB	306	CHL	C3A-C2A-CAA-CBA
23	AB	307	CHL	CBD-CGD-O2D-CED
23	Au	601	CHL	C2-C3-C5-C6
23	Au	601	CHL	C4-C3-C5-C6
23	Au	605	CHL	C3A-C2A-CAA-CBA
23	Au	606	CHL	C2B-C3B-CAB-CBB
23	Au	606	CHL	C4B-C3B-CAB-CBB
23	Au	607	CHL	C1A-C2A-CAA-CBA
23	Au	607	CHL	C3A-C2A-CAA-CBA
23	Au	608	CHL	C1A-C2A-CAA-CBA
23	Au	608	CHL	C3A-C2A-CAA-CBA
23	Au	608	CHL	C3C-C2C-CMC-OMC
23	Au	608	CHL	C14-C13-C15-C16
23	A2	601	CHL	C1A-C2A-CAA-CBA
23	A2	601	CHL	C3C-C2C-CMC-OMC
23	A2	605	CHL	C1A-C2A-CAA-CBA
23	A2	605	CHL	C3A-C2A-CAA-CBA
23	A2	606	CHL	C2B-C3B-CAB-CBB
23	A2	606	CHL	C4B-C3B-CAB-CBB
23	A2	606	CHL	C1C-C2C-CMC-OMC
23	A2	606	CHL	C3C-C2C-CMC-OMC
23	A2	606	CHL	CBD-CGD-O2D-CED
23	A2	607	CHL	C1A-C2A-CAA-CBA
23	A2	607	CHL	C3A-C2A-CAA-CBA
23	A2	608	CHL	C1A-C2A-CAA-CBA
23	A2	608	CHL	C3C-C2C-CMC-OMC
23	A2	608	CHL	CBD-CGD-O2D-CED
23	A6	601	CHL	C1C-C2C-CMC-OMC
23	A6	601	CHL	C3C-C2C-CMC-OMC
23	A6	605	CHL	C1C-C2C-CMC-OMC
23	A6	605	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
23	A6	606	CHL	CHA-CBD-CGD-O1D
23	A6	606	CHL	CHA-CBD-CGD-O2D
23	A6	607	CHL	C1A-C2A-CAA-CBA
23	A6	607	CHL	C3A-C2A-CAA-CBA
23	A6	607	CHL	C1C-C2C-CMC-OMC
23	A6	607	CHL	C3C-C2C-CMC-OMC
23	A6	607	CHL	C2C-C3C-CAC-CBC
23	A6	607	CHL	C4C-C3C-CAC-CBC
23	BB	302	CHL	C2-C3-C5-C6
23	BB	302	CHL	C4-C3-C5-C6
23	BB	306	CHL	C1A-C2A-CAA-CBA
23	BB	306	CHL	C3A-C2A-CAA-CBA
23	BB	307	CHL	C1A-C2A-CAA-CBA
23	BB	307	CHL	C3A-C2A-CAA-CBA
23	BB	307	CHL	C1C-C2C-CMC-OMC
23	BB	307	CHL	C3C-C2C-CMC-OMC
23	BB	307	CHL	CBD-CGD-O2D-CED
23	BB	308	CHL	C1A-C2A-CAA-CBA
23	BB	309	CHL	C1C-C2C-CMC-OMC
23	BB	309	CHL	C3C-C2C-CMC-OMC
23	BB	309	CHL	CBD-CGD-O2D-CED
23	BB	310	CHL	CHA-CBD-CGD-O1D
23	BB	310	CHL	CAD-CBD-CGD-O1D
23	BB	310	CHL	CAD-CBD-CGD-O2D
23	BB	310	CHL	C14-C13-C15-C16
23	BJ	601	CHL	C2-C3-C5-C6
23	BJ	601	CHL	C4-C3-C5-C6
23	BJ	605	CHL	CHA-CBD-CGD-O1D
23	BJ	605	CHL	CHA-CBD-CGD-O2D
23	BJ	605	CHL	CAD-CBD-CGD-O1D
23	BJ	606	CHL	C2B-C3B-CAB-CBB
23	BJ	606	CHL	C4B-C3B-CAB-CBB
23	BJ	607	CHL	C1A-C2A-CAA-CBA
23	BJ	608	CHL	C1A-C2A-CAA-CBA
23	BJ	608	CHL	C3A-C2A-CAA-CBA
23	BJ	608	CHL	C1C-C2C-CMC-OMC
23	BJ	608	CHL	C3C-C2C-CMC-OMC
23	BQ	601	CHL	CBD-CGD-O2D-CED
23	BQ	601	CHL	C4-C3-C5-C6
23	BQ	605	CHL	C1A-C2A-CAA-CBA
23	BQ	605	CHL	C3A-C2A-CAA-CBA
23	BQ	606	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	BQ	606	CHL	C4B-C3B-CAB-CBB
23	BQ	606	CHL	C1C-C2C-CMC-OMC
23	BQ	606	CHL	C3C-C2C-CMC-OMC
23	BQ	606	CHL	CBD-CGD-O2D-CED
23	BQ	607	CHL	C1A-C2A-CAA-CBA
23	BQ	607	CHL	C3A-C2A-CAA-CBA
23	BQ	608	CHL	C1A-C2A-CAA-CBA
23	BQ	608	CHL	C3C-C2C-CMC-OMC
23	BQ	608	CHL	CBD-CGD-O2D-CED
23	BQ	609	CHL	C1C-C2C-CMC-OMC
23	BQ	609	CHL	C3C-C2C-CMC-OMC
23	BV	601	CHL	C1C-C2C-CMC-OMC
23	BV	601	CHL	C3C-C2C-CMC-OMC
23	BV	605	CHL	C1C-C2C-CMC-OMC
23	BV	605	CHL	C3C-C2C-CMC-OMC
23	BV	605	CHL	CHA-CBD-CGD-O1D
23	BV	605	CHL	CHA-CBD-CGD-O2D
23	BV	605	CHL	CAD-CBD-CGD-O1D
23	BV	606	CHL	CHA-CBD-CGD-O1D
23	BV	606	CHL	CHA-CBD-CGD-O2D
23	BV	607	CHL	C1A-C2A-CAA-CBA
23	BV	607	CHL	C3A-C2A-CAA-CBA
23	Ba	306	CHL	C1A-C2A-CAA-CBA
23	Ba	306	CHL	C3A-C2A-CAA-CBA
23	Ba	307	CHL	C1C-C2C-CMC-OMC
23	Ba	307	CHL	C3C-C2C-CMC-OMC
23	Ba	307	CHL	CBD-CGD-O2D-CED
23	Ba	308	CHL	C1A-C2A-CAA-CBA
23	Ba	308	CHL	C3A-C2A-CAA-CBA
23	Ba	309	CHL	C3C-C2C-CMC-OMC
23	Ba	309	CHL	C14-C13-C15-C16
23	Ba	310	CHL	C3C-C2C-CMC-OMC
23	Ba	310	CHL	CAD-CBD-CGD-O1D
23	Ba	310	CHL	CBD-CGD-O2D-CED
23	BU	605	CHL	C1A-C2A-CAA-CBA
23	BU	605	CHL	C3A-C2A-CAA-CBA
23	BU	605	CHL	C1C-C2C-CMC-OMC
23	BU	605	CHL	C3-C5-C6-C7
23	BU	606	CHL	C3C-C2C-CMC-OMC
23	BU	607	CHL	C1A-C2A-CAA-CBA
23	BU	607	CHL	C3A-C2A-CAA-CBA
23	BU	607	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	BU	607	CHL	CHA-CBD-CGD-O2D
23	BU	607	CHL	CAD-CBD-CGD-O1D
24	5	604	CLA	C1A-C2A-CAA-CBA
24	5	604	CLA	C3A-C2A-CAA-CBA
24	5	604	CLA	CBD-CGD-O2D-CED
24	5	611	CLA	C1A-C2A-CAA-CBA
24	5	611	CLA	C3A-C2A-CAA-CBA
24	5	611	CLA	CBD-CGD-O2D-CED
24	5	612	CLA	CHA-CBD-CGD-O2D
24	5	613	CLA	CBD-CGD-O2D-CED
24	5	614	CLA	C1A-C2A-CAA-CBA
24	5	614	CLA	CBD-CGD-O2D-CED
24	6	602	CLA	C1A-C2A-CAA-CBA
24	6	602	CLA	C3A-C2A-CAA-CBA
24	6	603	CLA	CBD-CGD-O2D-CED
24	6	604	CLA	C1A-C2A-CAA-CBA
24	6	604	CLA	C3A-C2A-CAA-CBA
24	6	610	CLA	C2B-C3B-CAB-CBB
24	6	610	CLA	C4B-C3B-CAB-CBB
24	6	611	CLA	C1A-C2A-CAA-CBA
24	6	611	CLA	CAD-CBD-CGD-O2D
24	6	612	CLA	CBD-CGD-O2D-CED
24	6	613	CLA	C1A-C2A-CAA-CBA
24	6	614	CLA	C1A-C2A-CAA-CBA
24	6	614	CLA	C3A-C2A-CAA-CBA
24	7	305	CLA	C1A-C2A-CAA-CBA
24	7	305	CLA	C3A-C2A-CAA-CBA
24	7	311	CLA	C2B-C3B-CAB-CBB
24	7	311	CLA	C4B-C3B-CAB-CBB
24	7	312	CLA	C3A-C2A-CAA-CBA
24	7	312	CLA	CHA-CBD-CGD-O1D
24	7	312	CLA	CHA-CBD-CGD-O2D
24	7	312	CLA	CAD-CBD-CGD-O1D
24	7	314	CLA	C1A-C2A-CAA-CBA
24	7	314	CLA	CBD-CGD-O2D-CED
24	7	315	CLA	C2A-CAA-CBA-CGA
24	7	315	CLA	CBD-CGD-O2D-CED
24	8	301	CLA	C3A-C2A-CAA-CBA
24	8	303	CLA	C1A-C2A-CAA-CBA
24	8	303	CLA	C3A-C2A-CAA-CBA
24	8	308	CLA	C3A-C2A-CAA-CBA
24	8	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	C2-C3-C5-C6
24	B	602	CLA	C4-C3-C5-C6
24	B	603	CLA	C14-C13-C15-C16
24	B	604	CLA	C1A-C2A-CAA-CBA
24	B	604	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	CHA-CBD-CGD-O1D
24	B	604	CLA	CHA-CBD-CGD-O2D
24	B	605	CLA	C1A-C2A-CAA-CBA
24	B	605	CLA	C3A-C2A-CAA-CBA
24	B	605	CLA	C4-C3-C5-C6
24	B	606	CLA	CBD-CGD-O2D-CED
24	B	607	CLA	C1A-C2A-CAA-CBA
24	B	608	CLA	C1A-C2A-CAA-CBA
24	B	608	CLA	CBD-CGD-O2D-CED
24	B	609	CLA	C3A-C2A-CAA-CBA
24	B	609	CLA	CHA-CBD-CGD-O1D
24	B	609	CLA	CHA-CBD-CGD-O2D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	B	612	CLA	C3A-C2A-CAA-CBA
24	B	614	CLA	C1A-C2A-CAA-CBA
24	B	614	CLA	C3A-C2A-CAA-CBA
24	D	401	CLA	C1A-C2A-CAA-CBA
24	D	401	CLA	C3A-C2A-CAA-CBA
24	D	401	CLA	C2-C3-C5-C6
24	D	401	CLA	C4-C3-C5-C6
24	G	602	CLA	C1A-C2A-CAA-CBA
24	G	602	CLA	C3A-C2A-CAA-CBA
24	G	602	CLA	CBA-CGA-O2A-C1
24	G	602	CLA	O1A-CGA-O2A-C1
24	G	604	CLA	C1A-C2A-CAA-CBA
24	G	604	CLA	C3A-C2A-CAA-CBA
24	G	604	CLA	CBD-CGD-O2D-CED
24	G	610	CLA	C1A-C2A-CAA-CBA
24	G	610	CLA	C3A-C2A-CAA-CBA
24	G	611	CLA	C1A-C2A-CAA-CBA
24	G	611	CLA	C3A-C2A-CAA-CBA
24	G	611	CLA	C2-C3-C5-C6
24	G	611	CLA	C4-C3-C5-C6
24	G	613	CLA	CBD-CGD-O2D-CED
24	I	102	CLA	CHA-CBD-CGD-O1D
24	I	102	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	N	602	CLA	CHA-CBD-CGD-O2D
24	N	610	CLA	C1A-C2A-CAA-CBA
24	N	610	CLA	CBD-CGD-O2D-CED
24	N	611	CLA	C11-C10-C8-C9
24	N	613	CLA	CBD-CGD-O2D-CED
24	N	614	CLA	C1A-C2A-CAA-CBA
24	N	614	CLA	CBD-CGD-O2D-CED
24	S	602	CLA	C3A-C2A-CAA-CBA
24	S	603	CLA	CBD-CGD-O2D-CED
24	S	604	CLA	C1A-C2A-CAA-CBA
24	S	604	CLA	C2B-C3B-CAB-CBB
24	S	604	CLA	C4B-C3B-CAB-CBB
24	S	604	CLA	CBD-CGD-O2D-CED
24	S	608	CLA	C1A-C2A-CAA-CBA
24	S	608	CLA	C3A-C2A-CAA-CBA
24	S	608	CLA	CBD-CGD-O2D-CED
24	S	610	CLA	CBD-CGD-O2D-CED
24	S	613	CLA	CBD-CGD-O2D-CED
24	Y	305	CLA	C1A-C2A-CAA-CBA
24	Y	305	CLA	C3A-C2A-CAA-CBA
24	Y	312	CLA	C1A-C2A-CAA-CBA
24	Y	312	CLA	C3A-C2A-CAA-CBA
24	Y	312	CLA	CBD-CGD-O2D-CED
24	Y	312	CLA	C2-C3-C5-C6
24	Y	312	CLA	C4-C3-C5-C6
24	Y	314	CLA	CBD-CGD-O2D-CED
24	Y	315	CLA	CBD-CGD-O2D-CED
24	b	604	CLA	CBD-CGD-O2D-CED
24	b	605	CLA	C1A-C2A-CAA-CBA
24	b	605	CLA	C3A-C2A-CAA-CBA
24	b	605	CLA	CHA-CBD-CGD-O1D
24	b	605	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	C1A-C2A-CAA-CBA
24	b	606	CLA	C3A-C2A-CAA-CBA
24	b	606	CLA	CBD-CGD-O2D-CED
24	b	607	CLA	CBD-CGD-O2D-CED
24	b	608	CLA	C1A-C2A-CAA-CBA
24	b	608	CLA	C3A-C2A-CAA-CBA
24	b	609	CLA	C1A-C2A-CAA-CBA
24	b	609	CLA	CBD-CGD-O2D-CED
24	b	610	CLA	C3A-C2A-CAA-CBA
24	b	610	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	b	610	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	C3A-C2A-CAA-CBA
24	b	614	CLA	CBD-CGD-O2D-CED
24	b	615	CLA	C1A-C2A-CAA-CBA
24	b	615	CLA	C3A-C2A-CAA-CBA
24	b	617	CLA	CBD-CGD-O2D-CED
24	d	401	CLA	C1A-C2A-CAA-CBA
24	d	401	CLA	C3A-C2A-CAA-CBA
24	d	401	CLA	C2-C3-C5-C6
24	d	401	CLA	C4-C3-C5-C6
24	g	602	CLA	C1A-C2A-CAA-CBA
24	g	602	CLA	C3A-C2A-CAA-CBA
24	g	602	CLA	CBA-CGA-O2A-C1
24	g	602	CLA	O1A-CGA-O2A-C1
24	g	604	CLA	C1A-C2A-CAA-CBA
24	g	604	CLA	C3A-C2A-CAA-CBA
24	g	610	CLA	C1A-C2A-CAA-CBA
24	g	610	CLA	C3A-C2A-CAA-CBA
24	g	610	CLA	CBD-CGD-O2D-CED
24	g	611	CLA	C2-C3-C5-C6
24	g	611	CLA	C4-C3-C5-C6
24	g	612	CLA	CHA-CBD-CGD-O2D
24	g	613	CLA	CBD-CGD-O2D-CED
24	n	604	CLA	CBD-CGD-O2D-CED
24	n	610	CLA	C1A-C2A-CAA-CBA
24	n	610	CLA	C3A-C2A-CAA-CBA
24	n	610	CLA	CBA-CGA-O2A-C1
24	n	610	CLA	O1A-CGA-O2A-C1
24	n	611	CLA	C1A-C2A-CAA-CBA
24	n	612	CLA	CHA-CBD-CGD-O1D
24	n	612	CLA	CHA-CBD-CGD-O2D
24	n	613	CLA	CBD-CGD-O2D-CED
24	n	614	CLA	C1A-C2A-CAA-CBA
24	n	614	CLA	CBD-CGD-O2D-CED
24	n	614	CLA	O1D-CGD-O2D-CED
24	s	602	CLA	C1A-C2A-CAA-CBA
24	s	602	CLA	C3A-C2A-CAA-CBA
24	s	603	CLA	CBD-CGD-O2D-CED
24	s	608	CLA	C1A-C2A-CAA-CBA
24	s	608	CLA	C3A-C2A-CAA-CBA
24	s	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	s	610	CLA	CBD-CGD-O2D-CED
24	s	610	CLA	O1D-CGD-O2D-CED
24	s	611	CLA	CBD-CGD-O2D-CED
24	s	613	CLA	CBD-CGD-O2D-CED
24	y	303	CLA	CHA-CBD-CGD-O2D
24	y	305	CLA	C1A-C2A-CAA-CBA
24	y	305	CLA	C3A-C2A-CAA-CBA
24	y	305	CLA	C2A-CAA-CBA-CGA
24	y	311	CLA	CBD-CGD-O2D-CED
24	y	312	CLA	C1A-C2A-CAA-CBA
24	y	312	CLA	C3A-C2A-CAA-CBA
24	y	314	CLA	CBD-CGD-O2D-CED
24	y	315	CLA	CBD-CGD-O2D-CED
24	A	405	CLA	CHA-CBD-CGD-O1D
24	A	405	CLA	CBD-CGD-O2D-CED
24	A	406	CLA	C2A-CAA-CBA-CGA
24	C	502	CLA	C3A-C2A-CAA-CBA
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	C2-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	C	505	CLA	C1A-C2A-CAA-CBA
24	C	505	CLA	C3A-C2A-CAA-CBA
24	C	505	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	CBD-CGD-O2D-CED
24	C	507	CLA	C2B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	C1A-C2A-CAA-CBA
24	C	508	CLA	C3A-C2A-CAA-CBA
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C3A-C2A-CAA-CBA
24	C	513	CLA	CBD-CGD-O2D-CED
24	a	407	CLA	CBD-CGD-O2D-CED
24	c	502	CLA	C3A-C2A-CAA-CBA
24	c	503	CLA	C1A-C2A-CAA-CBA
24	c	504	CLA	C2-C3-C5-C6
24	c	504	CLA	C4-C3-C5-C6
24	c	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	505	CLA	C1A-C2A-CAA-CBA
24	c	505	CLA	C3A-C2A-CAA-CBA
24	c	505	CLA	CBD-CGD-O2D-CED
24	c	506	CLA	CHA-CBD-CGD-O1D
24	c	506	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CBD-CGD-O2D-CED
24	c	508	CLA	C2B-C3B-CAB-CBB
24	c	508	CLA	C4B-C3B-CAB-CBB
24	c	509	CLA	C1A-C2A-CAA-CBA
24	c	509	CLA	C3A-C2A-CAA-CBA
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CBD-CGD-O2D-CED
24	c	509	CLA	C2-C3-C5-C6
24	c	509	CLA	C4-C3-C5-C6
24	c	510	CLA	CBD-CGD-O2D-CED
24	c	511	CLA	CBD-CGD-O2D-CED
24	c	514	CLA	C1A-C2A-CAA-CBA
24	c	514	CLA	C3A-C2A-CAA-CBA
24	c	514	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	CBD-CGD-O2D-CED
24	r	601	CLA	CHA-CBD-CGD-O1D
24	r	601	CLA	CHA-CBD-CGD-O2D
24	r	601	CLA	CBD-CGD-O2D-CED
24	r	604	CLA	C1A-C2A-CAA-CBA
24	r	608	CLA	C1A-C2A-CAA-CBA
24	r	608	CLA	C3A-C2A-CAA-CBA
24	r	608	CLA	CBD-CGD-O2D-CED
24	r	609	CLA	C6-C7-C8-C9
24	r	610	CLA	C1A-C2A-CAA-CBA
24	r	610	CLA	C3A-C2A-CAA-CBA
24	r	610	CLA	C2B-C3B-CAB-CBB
24	r	610	CLA	C4B-C3B-CAB-CBB
24	r	610	CLA	CBD-CGD-O2D-CED
24	r	611	CLA	CBD-CGD-O2D-CED
24	r	614	CLA	C1A-C2A-CAA-CBA
24	r	614	CLA	C3A-C2A-CAA-CBA
24	r	614	CLA	CBD-CGD-O2D-CED
24	9	604	CLA	C1A-C2A-CAA-CBA
24	9	604	CLA	C3A-C2A-CAA-CBA
24	9	604	CLA	CBD-CGD-O2D-CED
24	9	610	CLA	C2B-C3B-CAB-CBB
24	9	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	9	611	CLA	C1A-C2A-CAA-CBA
24	9	611	CLA	C3A-C2A-CAA-CBA
24	9	611	CLA	CBD-CGD-O2D-CED
24	9	613	CLA	CBD-CGD-O2D-CED
24	9	614	CLA	C1A-C2A-CAA-CBA
24	0	602	CLA	C1A-C2A-CAA-CBA
24	0	602	CLA	C3A-C2A-CAA-CBA
24	0	603	CLA	CBD-CGD-O2D-CED
24	0	604	CLA	C1A-C2A-CAA-CBA
24	0	604	CLA	C3A-C2A-CAA-CBA
24	0	604	CLA	CHA-CBD-CGD-O1D
24	0	604	CLA	CHA-CBD-CGD-O2D
24	0	604	CLA	CBD-CGD-O2D-CED
24	0	610	CLA	C2B-C3B-CAB-CBB
24	0	610	CLA	C4B-C3B-CAB-CBB
24	0	611	CLA	C1A-C2A-CAA-CBA
24	0	611	CLA	C2B-C3B-CAB-CBB
24	0	611	CLA	CAD-CBD-CGD-O2D
24	0	612	CLA	CBD-CGD-O2D-CED
24	0	613	CLA	C1A-C2A-CAA-CBA
24	0	614	CLA	C1A-C2A-CAA-CBA
24	0	614	CLA	C3A-C2A-CAA-CBA
24	AA	305	CLA	C1A-C2A-CAA-CBA
24	AA	305	CLA	C3A-C2A-CAA-CBA
24	AA	311	CLA	C2B-C3B-CAB-CBB
24	AA	311	CLA	C4B-C3B-CAB-CBB
24	AA	312	CLA	C3A-C2A-CAA-CBA
24	AA	312	CLA	CHA-CBD-CGD-O1D
24	AA	312	CLA	CHA-CBD-CGD-O2D
24	AA	312	CLA	CAD-CBD-CGD-O1D
24	AA	314	CLA	C1A-C2A-CAA-CBA
24	AA	314	CLA	CBD-CGD-O2D-CED
24	AA	315	CLA	CBD-CGD-O2D-CED
24	AB	301	CLA	C3A-C2A-CAA-CBA
24	AB	303	CLA	C1A-C2A-CAA-CBA
24	AB	303	CLA	C3A-C2A-CAA-CBA
24	AB	308	CLA	C1A-C2A-CAA-CBA
24	AB	308	CLA	C3A-C2A-CAA-CBA
24	AB	310	CLA	C1A-C2A-CAA-CBA
24	v	602	CLA	CBD-CGD-O2D-CED
24	v	603	CLA	C14-C13-C15-C16
24	v	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	v	604	CLA	C3A-C2A-CAA-CBA
24	v	604	CLA	CHA-CBD-CGD-O1D
24	v	604	CLA	CHA-CBD-CGD-O2D
24	v	605	CLA	C1A-C2A-CAA-CBA
24	v	605	CLA	C3A-C2A-CAA-CBA
24	v	605	CLA	C4-C3-C5-C6
24	v	606	CLA	CBD-CGD-O2D-CED
24	v	607	CLA	C1A-C2A-CAA-CBA
24	v	608	CLA	C1A-C2A-CAA-CBA
24	v	608	CLA	CBD-CGD-O2D-CED
24	v	609	CLA	C3A-C2A-CAA-CBA
24	v	609	CLA	CHA-CBD-CGD-O1D
24	v	609	CLA	CHA-CBD-CGD-O2D
24	v	609	CLA	CAD-CBD-CGD-O1D
24	v	612	CLA	C3A-C2A-CAA-CBA
24	v	614	CLA	C1A-C2A-CAA-CBA
24	v	614	CLA	C3A-C2A-CAA-CBA
24	2	402	CLA	C1A-C2A-CAA-CBA
24	2	402	CLA	C3A-C2A-CAA-CBA
24	2	402	CLA	C2-C3-C5-C6
24	2	402	CLA	C4-C3-C5-C6
24	Au	602	CLA	C1A-C2A-CAA-CBA
24	Au	602	CLA	C3A-C2A-CAA-CBA
24	Au	602	CLA	CBA-CGA-O2A-C1
24	Au	602	CLA	O1A-CGA-O2A-C1
24	Au	604	CLA	C1A-C2A-CAA-CBA
24	Au	604	CLA	C3A-C2A-CAA-CBA
24	Au	604	CLA	CBD-CGD-O2D-CED
24	Au	610	CLA	C1A-C2A-CAA-CBA
24	Au	610	CLA	C3A-C2A-CAA-CBA
24	Au	611	CLA	C1A-C2A-CAA-CBA
24	Au	611	CLA	C3A-C2A-CAA-CBA
24	Au	611	CLA	C4-C3-C5-C6
24	Au	613	CLA	CBD-CGD-O2D-CED
24	Aw	102	CLA	CHA-CBD-CGD-O1D
24	Aw	102	CLA	CHA-CBD-CGD-O2D
24	A2	602	CLA	CHA-CBD-CGD-O2D
24	A2	610	CLA	C1A-C2A-CAA-CBA
24	A2	610	CLA	C3A-C2A-CAA-CBA
24	A2	610	CLA	CBD-CGD-O2D-CED
24	A2	611	CLA	C11-C10-C8-C9
24	A2	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A2	614	CLA	C1A-C2A-CAA-CBA
24	A2	614	CLA	C3A-C2A-CAA-CBA
24	A2	614	CLA	CBD-CGD-O2D-CED
24	A6	602	CLA	C3A-C2A-CAA-CBA
24	A6	603	CLA	CBD-CGD-O2D-CED
24	A6	604	CLA	C1A-C2A-CAA-CBA
24	A6	604	CLA	C2B-C3B-CAB-CBB
24	A6	604	CLA	C4B-C3B-CAB-CBB
24	A6	604	CLA	CBD-CGD-O2D-CED
24	A6	608	CLA	C1A-C2A-CAA-CBA
24	A6	608	CLA	C3A-C2A-CAA-CBA
24	A6	608	CLA	CBD-CGD-O2D-CED
24	A6	610	CLA	CBD-CGD-O2D-CED
24	A6	613	CLA	CBD-CGD-O2D-CED
24	BB	305	CLA	C1A-C2A-CAA-CBA
24	BB	305	CLA	C3A-C2A-CAA-CBA
24	BB	312	CLA	C1A-C2A-CAA-CBA
24	BB	312	CLA	C3A-C2A-CAA-CBA
24	BB	312	CLA	CBD-CGD-O2D-CED
24	BB	312	CLA	C2-C3-C5-C6
24	BB	312	CLA	C4-C3-C5-C6
24	BB	314	CLA	CBD-CGD-O2D-CED
24	BB	315	CLA	CBD-CGD-O2D-CED
24	BE	604	CLA	CBD-CGD-O2D-CED
24	BE	605	CLA	C1A-C2A-CAA-CBA
24	BE	605	CLA	C3A-C2A-CAA-CBA
24	BE	605	CLA	CHA-CBD-CGD-O1D
24	BE	605	CLA	CHA-CBD-CGD-O2D
24	BE	606	CLA	C1A-C2A-CAA-CBA
24	BE	606	CLA	C3A-C2A-CAA-CBA
24	BE	606	CLA	CBD-CGD-O2D-CED
24	BE	607	CLA	CBD-CGD-O2D-CED
24	BE	608	CLA	C1A-C2A-CAA-CBA
24	BE	608	CLA	C3A-C2A-CAA-CBA
24	BE	609	CLA	C1A-C2A-CAA-CBA
24	BE	609	CLA	CBD-CGD-O2D-CED
24	BE	610	CLA	C3A-C2A-CAA-CBA
24	BE	610	CLA	CHA-CBD-CGD-O1D
24	BE	610	CLA	CHA-CBD-CGD-O2D
24	BE	610	CLA	CAD-CBD-CGD-O1D
24	BE	612	CLA	CHA-CBD-CGD-O2D
24	BE	613	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	BE	614	CLA	CBD-CGD-O2D-CED
24	BE	615	CLA	C1A-C2A-CAA-CBA
24	BE	615	CLA	C3A-C2A-CAA-CBA
24	BE	617	CLA	CBD-CGD-O2D-CED
24	BG	401	CLA	C1A-C2A-CAA-CBA
24	BG	401	CLA	C3A-C2A-CAA-CBA
24	BG	401	CLA	C2-C3-C5-C6
24	BG	401	CLA	C4-C3-C5-C6
24	BJ	602	CLA	C1A-C2A-CAA-CBA
24	BJ	602	CLA	C3A-C2A-CAA-CBA
24	BJ	602	CLA	CBA-CGA-O2A-C1
24	BJ	602	CLA	O1A-CGA-O2A-C1
24	BJ	604	CLA	C1A-C2A-CAA-CBA
24	BJ	604	CLA	C3A-C2A-CAA-CBA
24	BJ	610	CLA	C1A-C2A-CAA-CBA
24	BJ	610	CLA	C3A-C2A-CAA-CBA
24	BJ	610	CLA	CBD-CGD-O2D-CED
24	BJ	611	CLA	C2-C3-C5-C6
24	BJ	611	CLA	C4-C3-C5-C6
24	BJ	612	CLA	CHA-CBD-CGD-O2D
24	BJ	613	CLA	CBD-CGD-O2D-CED
24	BQ	604	CLA	CBD-CGD-O2D-CED
24	BQ	610	CLA	C1A-C2A-CAA-CBA
24	BQ	610	CLA	CBA-CGA-O2A-C1
24	BQ	610	CLA	O1A-CGA-O2A-C1
24	BQ	611	CLA	C1A-C2A-CAA-CBA
24	BQ	612	CLA	CHA-CBD-CGD-O1D
24	BQ	612	CLA	CHA-CBD-CGD-O2D
24	BQ	613	CLA	CBD-CGD-O2D-CED
24	BQ	614	CLA	C1A-C2A-CAA-CBA
24	BQ	614	CLA	CBD-CGD-O2D-CED
24	BQ	614	CLA	O1D-CGD-O2D-CED
24	BV	602	CLA	C3A-C2A-CAA-CBA
24	BV	603	CLA	CBD-CGD-O2D-CED
24	BV	608	CLA	C1A-C2A-CAA-CBA
24	BV	608	CLA	C3A-C2A-CAA-CBA
24	BV	608	CLA	CBD-CGD-O2D-CED
24	BV	610	CLA	CBD-CGD-O2D-CED
24	BV	610	CLA	O1D-CGD-O2D-CED
24	BV	611	CLA	CBD-CGD-O2D-CED
24	BV	613	CLA	CBD-CGD-O2D-CED
24	Ba	303	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	Ba	305	CLA	C1A-C2A-CAA-CBA
24	Ba	305	CLA	C3A-C2A-CAA-CBA
24	Ba	311	CLA	CBD-CGD-O2D-CED
24	Ba	312	CLA	C1A-C2A-CAA-CBA
24	Ba	312	CLA	C3A-C2A-CAA-CBA
24	Ba	314	CLA	CBD-CGD-O2D-CED
24	Ba	315	CLA	CBD-CGD-O2D-CED
24	R	404	CLA	CHA-CBD-CGD-O1D
24	R	404	CLA	CBD-CGD-O2D-CED
24	R	405	CLA	C2A-CAA-CBA-CGA
24	1	502	CLA	C3A-C2A-CAA-CBA
24	1	502	CLA	CHA-CBD-CGD-O1D
24	1	502	CLA	CHA-CBD-CGD-O2D
24	1	504	CLA	C2-C3-C5-C6
24	1	504	CLA	C4-C3-C5-C6
24	1	505	CLA	C1A-C2A-CAA-CBA
24	1	505	CLA	C3A-C2A-CAA-CBA
24	1	505	CLA	CBD-CGD-O2D-CED
24	1	506	CLA	CBD-CGD-O2D-CED
24	1	507	CLA	C2B-C3B-CAB-CBB
24	1	507	CLA	C4B-C3B-CAB-CBB
24	1	508	CLA	C1A-C2A-CAA-CBA
24	1	508	CLA	C3A-C2A-CAA-CBA
24	1	508	CLA	CHA-CBD-CGD-O2D
24	1	508	CLA	C4-C3-C5-C6
24	1	513	CLA	C1A-C2A-CAA-CBA
24	1	513	CLA	C3A-C2A-CAA-CBA
24	1	513	CLA	CBD-CGD-O2D-CED
24	BF	502	CLA	C3A-C2A-CAA-CBA
24	BF	503	CLA	C1A-C2A-CAA-CBA
24	BF	504	CLA	C2-C3-C5-C6
24	BF	504	CLA	C4-C3-C5-C6
24	BF	505	CLA	C1A-C2A-CAA-CBA
24	BF	505	CLA	C3A-C2A-CAA-CBA
24	BF	505	CLA	CBD-CGD-O2D-CED
24	BF	506	CLA	CHA-CBD-CGD-O1D
24	BF	506	CLA	CHA-CBD-CGD-O2D
24	BF	506	CLA	CAD-CBD-CGD-O1D
24	BF	507	CLA	CBD-CGD-O2D-CED
24	BF	508	CLA	C2B-C3B-CAB-CBB
24	BF	508	CLA	C4B-C3B-CAB-CBB
24	BF	509	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	BF	509	CLA	C3A-C2A-CAA-CBA
24	BF	509	CLA	CHA-CBD-CGD-O2D
24	BF	509	CLA	C2-C3-C5-C6
24	BF	509	CLA	C4-C3-C5-C6
24	BF	511	CLA	CBD-CGD-O2D-CED
24	BF	512	CLA	C2B-C3B-CAB-CBB
24	BF	512	CLA	C4B-C3B-CAB-CBB
24	BF	514	CLA	C1A-C2A-CAA-CBA
24	BF	514	CLA	C3A-C2A-CAA-CBA
24	BF	514	CLA	CBD-CGD-O2D-CED
24	BU	601	CLA	CHA-CBD-CGD-O1D
24	BU	601	CLA	CHA-CBD-CGD-O2D
24	BU	604	CLA	C1A-C2A-CAA-CBA
24	BU	608	CLA	C1A-C2A-CAA-CBA
24	BU	608	CLA	C3A-C2A-CAA-CBA
24	BU	608	CLA	CBD-CGD-O2D-CED
24	BU	608	CLA	O1D-CGD-O2D-CED
24	BU	609	CLA	C6-C7-C8-C9
24	BU	610	CLA	C1A-C2A-CAA-CBA
24	BU	610	CLA	C3A-C2A-CAA-CBA
24	BU	610	CLA	C2B-C3B-CAB-CBB
24	BU	610	CLA	C4B-C3B-CAB-CBB
24	BU	610	CLA	CBD-CGD-O2D-CED
24	BU	611	CLA	CBD-CGD-O2D-CED
24	BU	614	CLA	C1A-C2A-CAA-CBA
24	BU	614	CLA	C3A-C2A-CAA-CBA
24	BU	614	CLA	CBD-CGD-O2D-CED
25	s	614	LUT	C7-C8-C9-C10
25	s	614	LUT	C7-C8-C9-C19
25	BV	614	LUT	C7-C8-C9-C10
25	BV	614	LUT	C7-C8-C9-C19
26	5	617	NEX	C12-C13-C14-C15
26	5	617	NEX	C20-C13-C14-C15
26	5	617	NEX	C14-C15-C35-C34
26	5	617	NEX	O24-C26-C27-C28
26	5	617	NEX	C31-C32-C33-C40
26	5	617	NEX	C32-C33-C34-C35
26	5	617	NEX	C40-C33-C34-C35
26	7	319	NEX	C7-C8-C9-C10
26	7	319	NEX	C11-C10-C9-C8
26	7	319	NEX	C11-C10-C9-C19
26	7	319	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	7	319	NEX	C10-C11-C12-C13
26	7	319	NEX	C11-C12-C13-C20
26	7	319	NEX	C14-C15-C35-C34
26	7	319	NEX	O24-C26-C27-C28
26	7	319	NEX	C27-C28-C29-C30
26	7	319	NEX	C27-C28-C29-C39
26	7	319	NEX	C28-C29-C30-C31
26	7	319	NEX	C39-C29-C30-C31
26	7	319	NEX	C31-C32-C33-C40
26	7	319	NEX	C32-C33-C34-C35
26	7	319	NEX	C40-C33-C34-C35
26	G	617	NEX	C7-C8-C9-C10
26	G	617	NEX	C7-C8-C9-C19
26	G	617	NEX	C11-C10-C9-C8
26	G	617	NEX	C11-C10-C9-C19
26	G	617	NEX	C10-C11-C12-C13
26	G	617	NEX	C11-C12-C13-C14
26	G	617	NEX	C11-C12-C13-C20
26	G	617	NEX	C12-C13-C14-C15
26	G	617	NEX	C20-C13-C14-C15
26	G	617	NEX	O24-C26-C27-C28
26	G	617	NEX	C28-C29-C30-C31
26	G	617	NEX	C39-C29-C30-C31
26	G	617	NEX	C32-C33-C34-C35
26	G	617	NEX	C40-C33-C34-C35
26	N	617	NEX	C14-C15-C35-C34
26	N	617	NEX	O24-C26-C27-C28
26	N	617	NEX	C27-C28-C29-C30
26	N	617	NEX	C27-C28-C29-C39
26	N	617	NEX	C31-C32-C33-C34
26	N	617	NEX	C31-C32-C33-C40
26	N	617	NEX	C32-C33-C34-C35
26	N	617	NEX	C40-C33-C34-C35
26	S	616	NEX	C7-C8-C9-C10
26	S	616	NEX	C11-C10-C9-C8
26	S	616	NEX	C10-C11-C12-C13
26	S	616	NEX	C27-C28-C29-C30
26	S	616	NEX	C27-C28-C29-C39
26	S	616	NEX	C32-C33-C34-C35
26	S	616	NEX	C40-C33-C34-C35
26	Y	318	NEX	C27-C28-C29-C30
26	Y	318	NEX	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
26	Y	318	NEX	C32-C33-C34-C35
26	Y	318	NEX	C40-C33-C34-C35
26	g	617	NEX	C7-C8-C9-C10
26	g	617	NEX	C11-C10-C9-C8
26	g	617	NEX	C11-C10-C9-C19
26	g	617	NEX	C9-C10-C11-C12
26	g	617	NEX	C10-C11-C12-C13
26	g	617	NEX	C12-C13-C14-C15
26	g	617	NEX	C20-C13-C14-C15
26	g	617	NEX	O24-C26-C27-C28
26	g	617	NEX	C30-C31-C32-C33
26	g	617	NEX	C32-C33-C34-C35
26	g	617	NEX	C40-C33-C34-C35
26	n	617	NEX	C20-C13-C14-C15
26	n	617	NEX	C14-C15-C35-C34
26	n	617	NEX	O24-C26-C27-C28
26	n	617	NEX	C27-C28-C29-C30
26	n	617	NEX	C27-C28-C29-C39
26	n	617	NEX	C31-C32-C33-C34
26	n	617	NEX	C31-C32-C33-C40
26	n	617	NEX	C32-C33-C34-C35
26	n	617	NEX	C40-C33-C34-C35
26	s	616	NEX	C7-C8-C9-C10
26	s	616	NEX	C10-C11-C12-C13
26	s	616	NEX	C13-C14-C15-C35
26	s	616	NEX	C27-C28-C29-C30
26	s	616	NEX	C27-C28-C29-C39
26	s	616	NEX	C32-C33-C34-C35
26	s	616	NEX	C40-C33-C34-C35
26	y	318	NEX	C14-C15-C35-C34
26	y	318	NEX	C27-C28-C29-C30
26	y	318	NEX	C27-C28-C29-C39
26	y	318	NEX	C32-C33-C34-C35
26	y	318	NEX	C40-C33-C34-C35
26	r	617	NEX	C11-C10-C9-C8
26	r	617	NEX	C11-C10-C9-C19
26	r	617	NEX	C12-C13-C14-C15
26	r	617	NEX	C20-C13-C14-C15
26	r	617	NEX	C27-C28-C29-C30
26	r	617	NEX	C27-C28-C29-C39
26	r	617	NEX	C28-C29-C30-C31
26	r	617	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	r	617	NEX	C30-C31-C32-C33
26	r	617	NEX	C32-C33-C34-C35
26	r	617	NEX	C40-C33-C34-C35
26	9	617	NEX	C12-C13-C14-C15
26	9	617	NEX	C20-C13-C14-C15
26	9	617	NEX	C14-C15-C35-C34
26	9	617	NEX	O24-C26-C27-C28
26	9	617	NEX	C32-C33-C34-C35
26	9	617	NEX	C40-C33-C34-C35
26	AA	319	NEX	C7-C8-C9-C10
26	AA	319	NEX	C11-C10-C9-C8
26	AA	319	NEX	C11-C10-C9-C19
26	AA	319	NEX	C9-C10-C11-C12
26	AA	319	NEX	C10-C11-C12-C13
26	AA	319	NEX	C11-C12-C13-C20
26	AA	319	NEX	C14-C15-C35-C34
26	AA	319	NEX	O24-C26-C27-C28
26	AA	319	NEX	C27-C28-C29-C30
26	AA	319	NEX	C27-C28-C29-C39
26	AA	319	NEX	C28-C29-C30-C31
26	AA	319	NEX	C39-C29-C30-C31
26	AA	319	NEX	C31-C32-C33-C40
26	AA	319	NEX	C32-C33-C34-C35
26	AA	319	NEX	C40-C33-C34-C35
26	Au	617	NEX	C7-C8-C9-C10
26	Au	617	NEX	C7-C8-C9-C19
26	Au	617	NEX	C11-C10-C9-C8
26	Au	617	NEX	C11-C10-C9-C19
26	Au	617	NEX	C10-C11-C12-C13
26	Au	617	NEX	C11-C12-C13-C20
26	Au	617	NEX	C12-C13-C14-C15
26	Au	617	NEX	C20-C13-C14-C15
26	Au	617	NEX	O24-C26-C27-C28
26	Au	617	NEX	C28-C29-C30-C31
26	Au	617	NEX	C39-C29-C30-C31
26	Au	617	NEX	C32-C33-C34-C35
26	Au	617	NEX	C40-C33-C34-C35
26	A2	617	NEX	C14-C15-C35-C34
26	A2	617	NEX	O24-C26-C27-C28
26	A2	617	NEX	C27-C28-C29-C30
26	A2	617	NEX	C27-C28-C29-C39
26	A2	617	NEX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	A2	617	NEX	C31-C32-C33-C40
26	A2	617	NEX	C32-C33-C34-C35
26	A2	617	NEX	C40-C33-C34-C35
26	A6	616	NEX	C7-C8-C9-C10
26	A6	616	NEX	C11-C10-C9-C8
26	A6	616	NEX	C11-C10-C9-C19
26	A6	616	NEX	C10-C11-C12-C13
26	A6	616	NEX	C27-C28-C29-C30
26	A6	616	NEX	C27-C28-C29-C39
26	A6	616	NEX	C32-C33-C34-C35
26	A6	616	NEX	C40-C33-C34-C35
26	BB	318	NEX	C27-C28-C29-C30
26	BB	318	NEX	C27-C28-C29-C39
26	BB	320	NEX	C11-C10-C9-C8
26	BB	320	NEX	C11-C10-C9-C19
26	BB	320	NEX	C11-C12-C13-C20
26	BB	320	NEX	C12-C13-C14-C15
26	BB	320	NEX	C20-C13-C14-C15
26	BB	320	NEX	C27-C28-C29-C30
26	BB	320	NEX	C27-C28-C29-C39
26	BB	320	NEX	C28-C29-C30-C31
26	BB	320	NEX	C39-C29-C30-C31
26	BB	320	NEX	C30-C31-C32-C33
26	BB	320	NEX	C32-C33-C34-C35
26	BB	320	NEX	C40-C33-C34-C35
26	BJ	617	NEX	C7-C8-C9-C10
26	BJ	617	NEX	C11-C10-C9-C8
26	BJ	617	NEX	C11-C10-C9-C19
26	BJ	617	NEX	C9-C10-C11-C12
26	BJ	617	NEX	C10-C11-C12-C13
26	BJ	617	NEX	C12-C13-C14-C15
26	BJ	617	NEX	C20-C13-C14-C15
26	BJ	617	NEX	O24-C26-C27-C28
26	BJ	617	NEX	C30-C31-C32-C33
26	BJ	617	NEX	C32-C33-C34-C35
26	BJ	617	NEX	C40-C33-C34-C35
26	BQ	617	NEX	C11-C12-C13-C14
26	BQ	617	NEX	C11-C12-C13-C20
26	BQ	617	NEX	C12-C13-C14-C15
26	BQ	617	NEX	C20-C13-C14-C15
26	BQ	617	NEX	C14-C15-C35-C34
26	BQ	617	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	BQ	617	NEX	C27-C28-C29-C30
26	BQ	617	NEX	C27-C28-C29-C39
26	BQ	617	NEX	C31-C32-C33-C40
26	BV	616	NEX	C7-C8-C9-C10
26	BV	616	NEX	C10-C11-C12-C13
26	BV	616	NEX	C13-C14-C15-C35
26	BV	616	NEX	C27-C28-C29-C30
26	BV	616	NEX	C27-C28-C29-C39
26	BV	616	NEX	C32-C33-C34-C35
26	BV	616	NEX	C40-C33-C34-C35
26	Ba	318	NEX	C14-C15-C35-C34
26	Ba	318	NEX	C27-C28-C29-C30
26	Ba	318	NEX	C27-C28-C29-C39
26	Ba	318	NEX	C40-C33-C34-C35
27	5	618	LHG	O1-C1-C2-C3
27	5	618	LHG	C1-C2-C3-O3
27	5	618	LHG	C3-O3-P-O5
27	B	621	LHG	O1-C1-C2-O2
27	B	621	LHG	O1-C1-C2-C3
27	B	621	LHG	C3-O3-P-O5
27	B	621	LHG	C4-O6-P-O3
27	B	621	LHG	C4-O6-P-O4
27	B	621	LHG	C4-O6-P-O5
27	B	621	LHG	C24-C23-O8-C6
27	D	404	LHG	C4-O6-P-O4
27	L	102	LHG	C3-O3-P-O5
27	N	618	LHG	C1-C2-C3-O3
27	N	618	LHG	C3-O3-P-O5
27	N	618	LHG	C3-O3-P-O6
27	W	201	LHG	C3-O3-P-O4
27	W	201	LHG	C3-O3-P-O5
27	Y	319	LHG	C3-O3-P-O4
27	b	622	LHG	O1-C1-C2-C3
27	b	622	LHG	C3-O3-P-O5
27	b	622	LHG	C24-C23-O8-C6
27	b	624	LHG	O1-C1-C2-C3
27	b	624	LHG	C3-O3-P-O5
27	d	404	LHG	C4-O6-P-O4
27	n	618	LHG	C1-C2-C3-O3
27	w	201	LHG	C3-O3-P-O4
27	w	201	LHG	C3-O3-P-O5
27	y	319	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
27	C	520	LHG	C3-O3-P-O5
27	C	520	LHG	C4-O6-P-O5
27	C	521	LHG	O1-C1-C2-O2
27	C	521	LHG	C3-O3-P-O4
27	C	521	LHG	O7-C5-C6-O8
27	c	519	LHG	C3-O3-P-O5
27	c	519	LHG	C4-O6-P-O5
27	c	520	LHG	C3-O3-P-O4
27	r	618	LHG	C2-C3-O3-P
27	r	618	LHG	C3-O3-P-O4
27	9	618	LHG	O1-C1-C2-C3
27	9	618	LHG	C1-C2-C3-O3
27	9	618	LHG	C3-O3-P-O5
27	v	621	LHG	O1-C1-C2-O2
27	v	621	LHG	O1-C1-C2-C3
27	v	621	LHG	C3-O3-P-O5
27	v	621	LHG	C4-O6-P-O3
27	v	621	LHG	C4-O6-P-O4
27	v	621	LHG	C4-O6-P-O5
27	v	621	LHG	C24-C23-O8-C6
27	2	406	LHG	C4-O6-P-O4
27	Az	102	LHG	C3-O3-P-O5
27	A2	618	LHG	C1-C2-C3-O3
27	A2	618	LHG	C3-O3-P-O5
27	A2	618	LHG	C3-O3-P-O6
27	A0	202	LHG	C3-O3-P-O4
27	A0	202	LHG	C3-O3-P-O5
27	BB	319	LHG	C3-O3-P-O4
27	BE	622	LHG	O1-C1-C2-C3
27	BE	622	LHG	C3-O3-P-O5
27	BE	622	LHG	C24-C23-O8-C6
27	BE	624	LHG	O1-C1-C2-C3
27	BE	624	LHG	C3-O3-P-O5
27	BG	404	LHG	C4-O6-P-O4
27	BQ	618	LHG	C1-C2-C3-O3
27	BY	201	LHG	C3-O3-P-O4
27	BY	201	LHG	C3-O3-P-O5
27	Ba	319	LHG	C3-O3-P-O4
27	1	520	LHG	C3-O3-P-O5
27	1	520	LHG	C4-O6-P-O5
27	1	521	LHG	O1-C1-C2-O2
27	1	521	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
27	1	521	LHG	O7-C5-C6-O8
27	BF	520	LHG	C3-O3-P-O5
27	BF	520	LHG	C4-O6-P-O5
27	BF	521	LHG	C3-O3-P-O4
27	BU	617	LHG	C2-C3-O3-P
27	BU	617	LHG	C3-O3-P-O4
28	5	619	XAT	C7-C8-C9-C19
28	5	619	XAT	C10-C11-C12-C13
28	5	619	XAT	C12-C13-C14-C15
28	5	619	XAT	C14-C15-C35-C34
28	5	619	XAT	C26-C27-C28-C29
28	5	619	XAT	C27-C28-C29-C30
28	5	619	XAT	C39-C29-C30-C31
28	5	619	XAT	C31-C32-C33-C34
28	5	619	XAT	C40-C33-C34-C35
28	7	301	XAT	C11-C10-C9-C8
28	7	301	XAT	C12-C13-C14-C15
28	7	301	XAT	O24-C26-C27-C28
28	7	301	XAT	C27-C28-C29-C30
28	7	301	XAT	C39-C29-C30-C31
28	7	301	XAT	C40-C33-C34-C35
28	7	318	XAT	O4-C6-C7-C8
28	7	318	XAT	C7-C8-C9-C19
28	7	318	XAT	C11-C10-C9-C19
28	7	318	XAT	C10-C11-C12-C13
28	7	318	XAT	C12-C13-C14-C15
28	7	318	XAT	O24-C26-C27-C28
28	7	318	XAT	C27-C28-C29-C30
28	7	318	XAT	C39-C29-C30-C31
28	7	318	XAT	C29-C30-C31-C32
28	7	318	XAT	C31-C32-C33-C40
28	7	318	XAT	C40-C33-C34-C35
28	8	312	XAT	O4-C6-C7-C8
28	8	312	XAT	C6-C7-C8-C9
28	8	312	XAT	C7-C8-C9-C19
28	8	312	XAT	C11-C10-C9-C19
28	8	312	XAT	C11-C12-C13-C14
28	8	312	XAT	C11-C12-C13-C20
28	8	312	XAT	C12-C13-C14-C15
28	8	312	XAT	O24-C26-C27-C28
28	8	312	XAT	C27-C28-C29-C39
28	8	312	XAT	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	8	312	XAT	C29-C30-C31-C32
28	8	312	XAT	C30-C31-C32-C33
28	8	312	XAT	C31-C32-C33-C40
28	8	312	XAT	C40-C33-C34-C35
28	G	619	XAT	O4-C6-C7-C8
28	G	619	XAT	C6-C7-C8-C9
28	G	619	XAT	C11-C10-C9-C8
28	G	619	XAT	C10-C11-C12-C13
28	G	619	XAT	C27-C28-C29-C30
28	G	619	XAT	C39-C29-C30-C31
28	G	619	XAT	C31-C32-C33-C34
28	G	619	XAT	C40-C33-C34-C35
28	N	619	XAT	O4-C6-C7-C8
28	N	619	XAT	C6-C7-C8-C9
28	N	619	XAT	C7-C8-C9-C10
28	N	619	XAT	C7-C8-C9-C19
28	N	619	XAT	C11-C10-C9-C8
28	N	619	XAT	C10-C11-C12-C13
28	N	619	XAT	C31-C32-C33-C40
28	N	619	XAT	C40-C33-C34-C35
28	Y	301	XAT	O4-C6-C7-C8
28	Y	301	XAT	C6-C7-C8-C9
28	Y	301	XAT	C11-C10-C9-C8
28	Y	301	XAT	C10-C11-C12-C13
28	Y	301	XAT	C12-C13-C14-C15
28	Y	301	XAT	C27-C28-C29-C30
28	Y	301	XAT	C39-C29-C30-C31
28	Y	301	XAT	C31-C32-C33-C40
28	Y	301	XAT	C40-C33-C34-C35
28	g	619	XAT	O4-C6-C7-C8
28	g	619	XAT	C6-C7-C8-C9
28	g	619	XAT	C11-C10-C9-C8
28	g	619	XAT	C10-C11-C12-C13
28	g	619	XAT	C12-C13-C14-C15
28	g	619	XAT	C27-C28-C29-C30
28	g	619	XAT	C39-C29-C30-C31
28	g	619	XAT	C31-C32-C33-C34
28	g	619	XAT	C40-C33-C34-C35
28	n	619	XAT	O4-C6-C7-C8
28	n	619	XAT	C6-C7-C8-C9
28	n	619	XAT	C7-C8-C9-C10
28	n	619	XAT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
28	n	619	XAT	C11-C10-C9-C8
28	n	619	XAT	C10-C11-C12-C13
28	n	619	XAT	C11-C12-C13-C20
28	n	619	XAT	C27-C28-C29-C39
28	n	619	XAT	C40-C33-C34-C35
28	y	301	XAT	O4-C6-C7-C8
28	y	301	XAT	C6-C7-C8-C9
28	y	301	XAT	C7-C8-C9-C10
28	y	301	XAT	C7-C8-C9-C19
28	y	301	XAT	C11-C10-C9-C8
28	y	301	XAT	C20-C13-C14-C15
28	y	301	XAT	O24-C26-C27-C28
28	y	301	XAT	C27-C28-C29-C30
28	y	301	XAT	C39-C29-C30-C31
28	y	301	XAT	C31-C32-C33-C40
28	y	301	XAT	C40-C33-C34-C35
28	r	616	XAT	C7-C8-C9-C19
28	r	616	XAT	C11-C10-C9-C8
28	r	616	XAT	C11-C10-C9-C19
28	r	616	XAT	C10-C11-C12-C13
28	r	616	XAT	C12-C13-C14-C15
28	r	616	XAT	O24-C26-C27-C28
28	r	616	XAT	C27-C28-C29-C30
28	r	616	XAT	C27-C28-C29-C39
28	r	616	XAT	C40-C33-C34-C35
28	9	619	XAT	C7-C8-C9-C19
28	9	619	XAT	C10-C11-C12-C13
28	9	619	XAT	C13-C14-C15-C35
28	9	619	XAT	C26-C27-C28-C29
28	9	619	XAT	C27-C28-C29-C30
28	9	619	XAT	C39-C29-C30-C31
28	9	619	XAT	C40-C33-C34-C35
28	9	619	XAT	C33-C34-C35-C15
28	AA	301	XAT	C11-C10-C9-C8
28	AA	301	XAT	C12-C13-C14-C15
28	AA	301	XAT	O24-C26-C27-C28
28	AA	301	XAT	C27-C28-C29-C30
28	AA	301	XAT	C39-C29-C30-C31
28	AA	301	XAT	C40-C33-C34-C35
28	AA	318	XAT	O4-C6-C7-C8
28	AA	318	XAT	C7-C8-C9-C19
28	AA	318	XAT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
28	AA	318	XAT	C10-C11-C12-C13
28	AA	318	XAT	C12-C13-C14-C15
28	AA	318	XAT	O24-C26-C27-C28
28	AA	318	XAT	C27-C28-C29-C30
28	AA	318	XAT	C39-C29-C30-C31
28	AA	318	XAT	C29-C30-C31-C32
28	AA	318	XAT	C31-C32-C33-C40
28	AA	318	XAT	C40-C33-C34-C35
28	AB	312	XAT	O4-C6-C7-C8
28	AB	312	XAT	C6-C7-C8-C9
28	AB	312	XAT	C7-C8-C9-C19
28	AB	312	XAT	C11-C10-C9-C19
28	AB	312	XAT	C11-C12-C13-C14
28	AB	312	XAT	C11-C12-C13-C20
28	AB	312	XAT	C12-C13-C14-C15
28	AB	312	XAT	O24-C26-C27-C28
28	AB	312	XAT	C27-C28-C29-C39
28	AB	312	XAT	C39-C29-C30-C31
28	AB	312	XAT	C29-C30-C31-C32
28	AB	312	XAT	C30-C31-C32-C33
28	AB	312	XAT	C31-C32-C33-C40
28	AB	312	XAT	C40-C33-C34-C35
28	Au	619	XAT	O4-C6-C7-C8
28	Au	619	XAT	C6-C7-C8-C9
28	Au	619	XAT	C11-C10-C9-C8
28	Au	619	XAT	C10-C11-C12-C13
28	Au	619	XAT	C27-C28-C29-C30
28	Au	619	XAT	C39-C29-C30-C31
28	Au	619	XAT	C31-C32-C33-C34
28	Au	619	XAT	C40-C33-C34-C35
28	A2	619	XAT	O4-C6-C7-C8
28	A2	619	XAT	C6-C7-C8-C9
28	A2	619	XAT	C7-C8-C9-C10
28	A2	619	XAT	C7-C8-C9-C19
28	A2	619	XAT	C11-C10-C9-C8
28	A2	619	XAT	C10-C11-C12-C13
28	A2	619	XAT	C31-C32-C33-C40
28	A2	619	XAT	C40-C33-C34-C35
28	BB	301	XAT	O4-C6-C7-C8
28	BB	301	XAT	C6-C7-C8-C9
28	BB	301	XAT	C11-C10-C9-C8
28	BB	301	XAT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	BB	301	XAT	C12-C13-C14-C15
28	BB	301	XAT	C27-C28-C29-C30
28	BB	301	XAT	C39-C29-C30-C31
28	BB	301	XAT	C31-C32-C33-C40
28	BB	301	XAT	C40-C33-C34-C35
28	BJ	619	XAT	O4-C6-C7-C8
28	BJ	619	XAT	C6-C7-C8-C9
28	BJ	619	XAT	C11-C10-C9-C8
28	BJ	619	XAT	C10-C11-C12-C13
28	BJ	619	XAT	C12-C13-C14-C15
28	BJ	619	XAT	C27-C28-C29-C30
28	BJ	619	XAT	C39-C29-C30-C31
28	BJ	619	XAT	C31-C32-C33-C34
28	BJ	619	XAT	C40-C33-C34-C35
28	BQ	619	XAT	O4-C6-C7-C8
28	BQ	619	XAT	C6-C7-C8-C9
28	BQ	619	XAT	C7-C8-C9-C10
28	BQ	619	XAT	C7-C8-C9-C19
28	BQ	619	XAT	C11-C10-C9-C8
28	BQ	619	XAT	C10-C11-C12-C13
28	BQ	619	XAT	C11-C12-C13-C20
28	BQ	619	XAT	C27-C28-C29-C39
28	BQ	619	XAT	C40-C33-C34-C35
28	Ba	301	XAT	O4-C6-C7-C8
28	Ba	301	XAT	C6-C7-C8-C9
28	Ba	301	XAT	C7-C8-C9-C10
28	Ba	301	XAT	C7-C8-C9-C19
28	Ba	301	XAT	C11-C10-C9-C8
28	Ba	301	XAT	C20-C13-C14-C15
28	Ba	301	XAT	O24-C26-C27-C28
28	Ba	301	XAT	C27-C28-C29-C30
28	Ba	301	XAT	C39-C29-C30-C31
28	Ba	301	XAT	C31-C32-C33-C40
28	Ba	301	XAT	C40-C33-C34-C35
28	BU	616	XAT	C7-C8-C9-C19
28	BU	616	XAT	C11-C10-C9-C8
28	BU	616	XAT	C11-C10-C9-C19
28	BU	616	XAT	C10-C11-C12-C13
28	BU	616	XAT	C12-C13-C14-C15
28	BU	616	XAT	O24-C26-C27-C28
28	BU	616	XAT	C27-C28-C29-C30
28	BU	616	XAT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
28	BU	616	XAT	C40-C33-C34-C35
29	8	313	BCR	C1-C6-C7-C8
29	8	313	BCR	C7-C8-C9-C10
29	8	313	BCR	C7-C8-C9-C34
29	8	313	BCR	C18-C19-C20-C21
29	8	313	BCR	C20-C21-C22-C37
29	8	313	BCR	C37-C22-C23-C24
29	8	313	BCR	C22-C23-C24-C25
29	B	617	BCR	C21-C22-C23-C24
29	B	618	BCR	C7-C8-C9-C34
29	B	623	BCR	C6-C7-C8-C9
29	B	623	BCR	C21-C22-C23-C24
29	B	623	BCR	C37-C22-C23-C24
29	F	101	BCR	C7-C8-C9-C10
29	F	101	BCR	C7-C8-C9-C34
29	H	101	BCR	C1-C6-C7-C8
29	K	101	BCR	C1-C6-C7-C8
29	K	101	BCR	C21-C22-C23-C24
29	K	102	BCR	C7-C8-C9-C10
29	K	102	BCR	C7-C8-C9-C34
29	b	601	BCR	C7-C8-C9-C34
29	b	601	BCR	C11-C12-C13-C35
29	b	601	BCR	C14-C15-C16-C17
29	b	601	BCR	C21-C22-C23-C24
29	b	601	BCR	C37-C22-C23-C24
29	b	618	BCR	C22-C23-C24-C25
29	b	619	BCR	C7-C8-C9-C10
29	b	619	BCR	C7-C8-C9-C34
29	f	101	BCR	C7-C8-C9-C10
29	f	101	BCR	C7-C8-C9-C34
29	f	101	BCR	C11-C12-C13-C35
29	k	101	BCR	C1-C6-C7-C8
29	k	101	BCR	C21-C22-C23-C24
29	z	102	BCR	C1-C6-C7-C8
29	z	102	BCR	C7-C8-C9-C10
29	z	102	BCR	C7-C8-C9-C34
29	a	411	BCR	C23-C24-C25-C30
29	c	515	BCR	C20-C21-C22-C37
29	AB	313	BCR	C1-C6-C7-C8
29	AB	313	BCR	C7-C8-C9-C10
29	AB	313	BCR	C7-C8-C9-C34
29	AB	313	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	AB	313	BCR	C18-C19-C20-C21
29	AB	313	BCR	C20-C21-C22-C37
29	AB	313	BCR	C37-C22-C23-C24
29	AB	313	BCR	C22-C23-C24-C25
29	v	617	BCR	C21-C22-C23-C24
29	v	618	BCR	C7-C8-C9-C34
29	v	619	BCR	C14-C15-C16-C17
29	v	622	BCR	C6-C7-C8-C9
29	v	622	BCR	C7-C8-C9-C10
29	v	622	BCR	C21-C22-C23-C24
29	v	622	BCR	C37-C22-C23-C24
29	4	101	BCR	C7-C8-C9-C10
29	4	101	BCR	C7-C8-C9-C34
29	Ay	101	BCR	C21-C22-C23-C24
29	Ay	102	BCR	C1-C6-C7-C8
29	Ay	102	BCR	C7-C8-C9-C10
29	Ay	102	BCR	C7-C8-C9-C34
29	BE	601	BCR	C7-C8-C9-C34
29	BE	601	BCR	C11-C12-C13-C35
29	BE	601	BCR	C14-C15-C16-C17
29	BE	601	BCR	C21-C22-C23-C24
29	BE	601	BCR	C37-C22-C23-C24
29	BE	618	BCR	C22-C23-C24-C25
29	BE	619	BCR	C7-C8-C9-C10
29	BE	619	BCR	C7-C8-C9-C34
29	BI	101	BCR	C7-C8-C9-C10
29	BI	101	BCR	C7-C8-C9-C34
29	BI	101	BCR	C11-C12-C13-C35
29	BN	101	BCR	C1-C6-C7-C8
29	BN	101	BCR	C7-C8-C9-C10
29	BN	101	BCR	C21-C22-C23-C24
29	Bb	101	BCR	C1-C6-C7-C8
29	Bb	101	BCR	C7-C8-C9-C10
29	R	410	BCR	C7-C8-C9-C34
29	1	514	BCR	C1-C6-C7-C8
29	BD	411	BCR	C23-C24-C25-C30
29	BF	516	BCR	C20-C21-C22-C37
29	BF	516	BCR	C23-C24-C25-C30
30	B	624	LMG	O6-C1-O1-C7
30	i	101	LMG	C2-C1-O1-C7
30	i	101	LMG	O6-C1-O1-C7
30	A	412	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
30	A	412	LMG	O6-C1-O1-C7
30	C	519	LMG	C2-C1-O1-C7
30	C	519	LMG	O6-C1-O1-C7
30	c	518	LMG	C2-C1-O1-C7
30	c	518	LMG	O6-C1-O1-C7
30	v	623	LMG	O6-C1-O1-C7
30	A0	201	LMG	C2-C1-O1-C7
30	A0	201	LMG	O6-C1-O1-C7
30	BL	101	LMG	C2-C1-O1-C7
30	BL	101	LMG	O6-C1-O1-C7
30	1	519	LMG	C2-C1-O1-C7
30	1	519	LMG	O6-C1-O1-C7
30	BF	519	LMG	C2-C1-O1-C7
30	BF	519	LMG	O6-C1-O1-C7
31	d	403	PL9	C27-C28-C29-C31
32	D	406	SQD	C8-C7-O47-C45
32	D	406	SQD	O5-C5-C6-S
32	L	101	SQD	C2-C1-O6-C44
32	L	101	SQD	O49-C7-O47-C45
32	L	101	SQD	C8-C7-O47-C45
32	L	103	SQD	O5-C1-O6-C44
32	L	103	SQD	C8-C7-O47-C45
32	d	406	SQD	C8-C7-O47-C45
32	d	406	SQD	O5-C5-C6-S
32	l	101	SQD	O5-C1-O6-C44
32	l	101	SQD	C8-C7-O47-C45
32	l	102	SQD	C2-C1-O6-C44
32	l	102	SQD	O5-C1-O6-C44
32	l	102	SQD	O49-C7-O47-C45
32	l	102	SQD	C8-C7-O47-C45
32	A	413	SQD	C2-C1-O6-C44
32	a	412	SQD	C2-C1-O6-C44
32	2	408	SQD	C8-C7-O47-C45
32	2	408	SQD	O5-C5-C6-S
32	Az	101	SQD	C2-C1-O6-C44
32	Az	101	SQD	O5-C1-O6-C44
32	Az	101	SQD	O49-C7-O47-C45
32	Az	101	SQD	C8-C7-O47-C45
32	A1	101	SQD	O5-C1-O6-C44
32	A1	101	SQD	C8-C7-O47-C45
32	BG	406	SQD	C8-C7-O47-C45
32	BG	406	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
32	BO	101	SQD	O5-C1-O6-C44
32	BO	101	SQD	C8-C7-O47-C45
32	BO	102	SQD	C2-C1-O6-C44
32	BO	102	SQD	O5-C1-O6-C44
32	BO	102	SQD	O49-C7-O47-C45
32	BO	102	SQD	C8-C7-O47-C45
32	R	411	SQD	C2-C1-O6-C44
32	BD	412	SQD	C2-C1-O6-C44
33	f	102	HEM	C3D-CAD-CBD-CGD
34	H	102	DGD	C4D-C5D-C6D-O5D
34	H	102	DGD	C2E-C1E-O5D-C6D
34	H	102	DGD	O6E-C1E-O5D-C6D
34	h	102	DGD	C4D-C5D-C6D-O5D
34	A	402	DGD	C2D-C1D-O3G-C3G
34	A	402	DGD	O6D-C1D-O3G-C3G
34	C	517	DGD	C2D-C1D-O3G-C3G
34	C	517	DGD	O6D-C1D-O3G-C3G
34	C	517	DGD	C2E-C1E-O5D-C6D
34	C	517	DGD	O6E-C1E-O5D-C6D
34	a	401	DGD	C2D-C1D-O3G-C3G
34	a	401	DGD	O6D-C1D-O3G-C3G
34	c	517	DGD	C2D-C1D-O3G-C3G
34	c	517	DGD	O6D-C1D-O3G-C3G
34	c	517	DGD	C2E-C1E-O5D-C6D
34	c	517	DGD	O6E-C1E-O5D-C6D
34	Av	102	DGD	C4D-C5D-C6D-O5D
34	Av	102	DGD	C2E-C1E-O5D-C6D
34	Av	102	DGD	O6E-C1E-O5D-C6D
34	BK	102	DGD	C4D-C5D-C6D-O5D
34	R	401	DGD	C2D-C1D-O3G-C3G
34	R	401	DGD	O6D-C1D-O3G-C3G
34	1	517	DGD	C2D-C1D-O3G-C3G
34	1	517	DGD	O6D-C1D-O3G-C3G
34	1	517	DGD	C2E-C1E-O5D-C6D
34	1	517	DGD	O6E-C1E-O5D-C6D
34	BD	401	DGD	C2D-C1D-O3G-C3G
34	BD	401	DGD	O6D-C1D-O3G-C3G
34	BF	518	DGD	C2D-C1D-O3G-C3G
34	BF	518	DGD	O6D-C1D-O3G-C3G
34	BF	518	DGD	C2E-C1E-O5D-C6D
34	BF	518	DGD	O6E-C1E-O5D-C6D
38	a	409	PHO	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	5	601	CHL	O1D-CGD-O2D-CED
23	n	609	CHL	O1D-CGD-O2D-CED
23	y	310	CHL	O1D-CGD-O2D-CED
23	9	601	CHL	O1D-CGD-O2D-CED
23	BQ	609	CHL	O1D-CGD-O2D-CED
24	5	613	CLA	O1D-CGD-O2D-CED
24	7	315	CLA	O1D-CGD-O2D-CED
24	B	605	CLA	O1D-CGD-O2D-CED
24	B	608	CLA	O1D-CGD-O2D-CED
24	B	613	CLA	O1D-CGD-O2D-CED
24	G	610	CLA	O1D-CGD-O2D-CED
24	G	613	CLA	O1D-CGD-O2D-CED
24	Y	312	CLA	O1D-CGD-O2D-CED
24	Y	315	CLA	O1D-CGD-O2D-CED
24	b	606	CLA	O1D-CGD-O2D-CED
24	b	607	CLA	O1D-CGD-O2D-CED
24	g	613	CLA	O1D-CGD-O2D-CED
24	s	613	CLA	O1D-CGD-O2D-CED
24	C	508	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	O1D-CGD-O2D-CED
24	c	510	CLA	O1D-CGD-O2D-CED
24	r	601	CLA	O1D-CGD-O2D-CED
24	r	610	CLA	O1D-CGD-O2D-CED
24	r	614	CLA	O1D-CGD-O2D-CED
24	9	613	CLA	O1D-CGD-O2D-CED
24	AA	315	CLA	O1D-CGD-O2D-CED
24	v	605	CLA	O1D-CGD-O2D-CED
24	v	608	CLA	O1D-CGD-O2D-CED
24	v	613	CLA	O1D-CGD-O2D-CED
24	Au	610	CLA	O1D-CGD-O2D-CED
24	Au	613	CLA	O1D-CGD-O2D-CED
24	BB	315	CLA	O1D-CGD-O2D-CED
24	BE	607	CLA	O1D-CGD-O2D-CED
24	BJ	613	CLA	O1D-CGD-O2D-CED
24	BV	613	CLA	O1D-CGD-O2D-CED
24	1	508	CLA	O1D-CGD-O2D-CED
24	1	509	CLA	O1D-CGD-O2D-CED
24	BF	509	CLA	O1D-CGD-O2D-CED
24	BF	510	CLA	O1D-CGD-O2D-CED
24	BF	514	CLA	O1D-CGD-O2D-CED
24	BU	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	BU	609	CLA	O1D-CGD-O2D-CED
24	BU	610	CLA	O1D-CGD-O2D-CED
24	BU	614	CLA	O1D-CGD-O2D-CED
23	5	605	CHL	O1D-CGD-O2D-CED
23	9	605	CHL	O1D-CGD-O2D-CED
24	5	610	CLA	O1D-CGD-O2D-CED
24	6	611	CLA	O1D-CGD-O2D-CED
24	7	314	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	O1D-CGD-O2D-CED
24	N	613	CLA	O1D-CGD-O2D-CED
24	S	610	CLA	O1D-CGD-O2D-CED
24	S	613	CLA	O1D-CGD-O2D-CED
24	Y	314	CLA	O1D-CGD-O2D-CED
24	b	604	CLA	O1D-CGD-O2D-CED
24	b	614	CLA	O1D-CGD-O2D-CED
24	g	610	CLA	O1D-CGD-O2D-CED
24	n	613	CLA	O1D-CGD-O2D-CED
24	s	603	CLA	O1D-CGD-O2D-CED
24	y	314	CLA	O1D-CGD-O2D-CED
24	y	315	CLA	O1D-CGD-O2D-CED
24	A	405	CLA	O1D-CGD-O2D-CED
24	C	505	CLA	O1D-CGD-O2D-CED
24	C	513	CLA	O1D-CGD-O2D-CED
24	c	505	CLA	O1D-CGD-O2D-CED
24	c	514	CLA	O1D-CGD-O2D-CED
24	r	609	CLA	O1D-CGD-O2D-CED
24	9	610	CLA	O1D-CGD-O2D-CED
24	0	611	CLA	O1D-CGD-O2D-CED
24	AA	314	CLA	O1D-CGD-O2D-CED
24	A2	613	CLA	O1D-CGD-O2D-CED
24	A6	610	CLA	O1D-CGD-O2D-CED
24	A6	613	CLA	O1D-CGD-O2D-CED
24	BB	314	CLA	O1D-CGD-O2D-CED
24	BE	604	CLA	O1D-CGD-O2D-CED
24	BE	606	CLA	O1D-CGD-O2D-CED
24	BE	614	CLA	O1D-CGD-O2D-CED
24	BJ	610	CLA	O1D-CGD-O2D-CED
24	BQ	613	CLA	O1D-CGD-O2D-CED
24	BV	603	CLA	O1D-CGD-O2D-CED
24	Ba	314	CLA	O1D-CGD-O2D-CED
24	Ba	315	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	R	404	CLA	O1D-CGD-O2D-CED
24	1	503	CLA	O1D-CGD-O2D-CED
24	1	505	CLA	O1D-CGD-O2D-CED
24	1	513	CLA	O1D-CGD-O2D-CED
24	BF	505	CLA	O1D-CGD-O2D-CED
23	5	605	CHL	CBD-CGD-O2D-CED
23	6	606	CHL	CBD-CGD-O2D-CED
23	7	309	CHL	CBD-CGD-O2D-CED
23	8	304	CHL	CBD-CGD-O2D-CED
23	G	606	CHL	CBD-CGD-O2D-CED
23	N	605	CHL	CBD-CGD-O2D-CED
23	Y	310	CHL	CBD-CGD-O2D-CED
23	g	606	CHL	CBD-CGD-O2D-CED
23	n	605	CHL	CBD-CGD-O2D-CED
23	n	609	CHL	CBD-CGD-O2D-CED
23	y	306	CHL	CBD-CGD-O2D-CED
23	y	309	CHL	CBD-CGD-O2D-CED
23	9	605	CHL	CBD-CGD-O2D-CED
23	0	606	CHL	CBD-CGD-O2D-CED
23	AA	309	CHL	CBD-CGD-O2D-CED
23	AB	304	CHL	CBD-CGD-O2D-CED
23	Au	606	CHL	CBD-CGD-O2D-CED
23	A2	605	CHL	CBD-CGD-O2D-CED
23	A6	607	CHL	CBD-CGD-O2D-CED
23	BJ	606	CHL	CBD-CGD-O2D-CED
23	BQ	605	CHL	CBD-CGD-O2D-CED
23	BQ	609	CHL	CBD-CGD-O2D-CED
23	BV	607	CHL	CBD-CGD-O2D-CED
23	Ba	306	CHL	CBD-CGD-O2D-CED
23	Ba	309	CHL	CBD-CGD-O2D-CED
24	5	603	CLA	CBD-CGD-O2D-CED
24	5	610	CLA	CBD-CGD-O2D-CED
24	5	612	CLA	CBD-CGD-O2D-CED
24	6	604	CLA	CBD-CGD-O2D-CED
24	6	610	CLA	CBD-CGD-O2D-CED
24	6	611	CLA	CBD-CGD-O2D-CED
24	7	303	CLA	CBD-CGD-O2D-CED
24	7	313	CLA	CBD-CGD-O2D-CED
24	8	302	CLA	CBD-CGD-O2D-CED
24	8	303	CLA	CBD-CGD-O2D-CED
24	8	308	CLA	CBD-CGD-O2D-CED
24	8	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CBD-CGD-O2D-CED
24	B	605	CLA	CBD-CGD-O2D-CED
24	B	609	CLA	CBD-CGD-O2D-CED
24	B	613	CLA	CBD-CGD-O2D-CED
24	B	614	CLA	CBD-CGD-O2D-CED
24	B	616	CLA	CBD-CGD-O2D-CED
24	G	603	CLA	CBD-CGD-O2D-CED
24	G	610	CLA	CBD-CGD-O2D-CED
24	N	604	CLA	CBD-CGD-O2D-CED
24	S	611	CLA	CBD-CGD-O2D-CED
24	Y	305	CLA	CBD-CGD-O2D-CED
24	Y	311	CLA	CBD-CGD-O2D-CED
24	b	603	CLA	CBD-CGD-O2D-CED
24	g	604	CLA	CBD-CGD-O2D-CED
24	n	610	CLA	CBD-CGD-O2D-CED
24	s	604	CLA	CBD-CGD-O2D-CED
24	s	609	CLA	CBD-CGD-O2D-CED
24	y	312	CLA	CBD-CGD-O2D-CED
24	C	503	CLA	CBD-CGD-O2D-CED
24	C	504	CLA	CBD-CGD-O2D-CED
24	C	507	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CBD-CGD-O2D-CED
24	C	510	CLA	CBD-CGD-O2D-CED
24	c	503	CLA	CBD-CGD-O2D-CED
24	c	504	CLA	CBD-CGD-O2D-CED
24	c	508	CLA	CBD-CGD-O2D-CED
24	r	609	CLA	CBD-CGD-O2D-CED
24	9	610	CLA	CBD-CGD-O2D-CED
24	9	614	CLA	CBD-CGD-O2D-CED
24	0	610	CLA	CBD-CGD-O2D-CED
24	0	611	CLA	CBD-CGD-O2D-CED
24	AA	303	CLA	CBD-CGD-O2D-CED
24	AA	304	CLA	CBD-CGD-O2D-CED
24	AA	313	CLA	CBD-CGD-O2D-CED
24	AB	302	CLA	CBD-CGD-O2D-CED
24	AB	303	CLA	CBD-CGD-O2D-CED
24	AB	308	CLA	CBD-CGD-O2D-CED
24	AB	310	CLA	CBD-CGD-O2D-CED
24	v	603	CLA	CBD-CGD-O2D-CED
24	v	605	CLA	CBD-CGD-O2D-CED
24	v	609	CLA	CBD-CGD-O2D-CED
24	v	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	v	614	CLA	CBD-CGD-O2D-CED
24	v	616	CLA	CBD-CGD-O2D-CED
24	Au	603	CLA	CBD-CGD-O2D-CED
24	Au	610	CLA	CBD-CGD-O2D-CED
24	A2	604	CLA	CBD-CGD-O2D-CED
24	A6	611	CLA	CBD-CGD-O2D-CED
24	BB	305	CLA	CBD-CGD-O2D-CED
24	BB	311	CLA	CBD-CGD-O2D-CED
24	BE	603	CLA	CBD-CGD-O2D-CED
24	BJ	604	CLA	CBD-CGD-O2D-CED
24	BQ	610	CLA	CBD-CGD-O2D-CED
24	BV	604	CLA	CBD-CGD-O2D-CED
24	BV	609	CLA	CBD-CGD-O2D-CED
24	Ba	312	CLA	CBD-CGD-O2D-CED
24	1	503	CLA	CBD-CGD-O2D-CED
24	1	504	CLA	CBD-CGD-O2D-CED
24	1	508	CLA	CBD-CGD-O2D-CED
24	1	509	CLA	CBD-CGD-O2D-CED
24	1	510	CLA	CBD-CGD-O2D-CED
24	BD	407	CLA	CBD-CGD-O2D-CED
24	BF	503	CLA	CBD-CGD-O2D-CED
24	BF	504	CLA	CBD-CGD-O2D-CED
24	BF	509	CLA	CBD-CGD-O2D-CED
24	BF	510	CLA	CBD-CGD-O2D-CED
24	BU	601	CLA	CBD-CGD-O2D-CED
24	BU	609	CLA	CBD-CGD-O2D-CED
23	6	609	CHL	O1A-CGA-O2A-C1
23	0	609	CHL	O1A-CGA-O2A-C1
24	N	610	CLA	O1A-CGA-O2A-C1
24	b	617	CLA	O1A-CGA-O2A-C1
24	A	407	CLA	O1A-CGA-O2A-C1
24	a	407	CLA	O1A-CGA-O2A-C1
24	r	610	CLA	O1A-CGA-O2A-C1
24	A2	610	CLA	O1A-CGA-O2A-C1
24	BE	617	CLA	O1A-CGA-O2A-C1
24	R	406	CLA	O1A-CGA-O2A-C1
24	BF	514	CLA	O1A-CGA-O2A-C1
24	BU	610	CLA	O1A-CGA-O2A-C1
27	B	621	LHG	O10-C23-O8-C6
27	b	622	LHG	O10-C23-O8-C6
27	v	621	LHG	O10-C23-O8-C6
27	BE	622	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
30	C	501	LMG	O10-C28-O8-C9
30	c	501	LMG	O10-C28-O8-C9
30	1	501	LMG	O10-C28-O8-C9
30	BF	501	LMG	O10-C28-O8-C9
23	7	309	CHL	O1D-CGD-O2D-CED
23	8	304	CHL	O1D-CGD-O2D-CED
23	8	305	CHL	O1D-CGD-O2D-CED
23	8	307	CHL	O1D-CGD-O2D-CED
23	n	601	CHL	O1D-CGD-O2D-CED
23	n	608	CHL	O1D-CGD-O2D-CED
23	y	307	CHL	O1D-CGD-O2D-CED
23	AB	304	CHL	O1D-CGD-O2D-CED
23	AB	305	CHL	O1D-CGD-O2D-CED
23	AB	307	CHL	O1D-CGD-O2D-CED
23	BQ	601	CHL	O1D-CGD-O2D-CED
23	BQ	608	CHL	O1D-CGD-O2D-CED
23	Ba	307	CHL	O1D-CGD-O2D-CED
24	5	604	CLA	O1D-CGD-O2D-CED
24	6	610	CLA	O1D-CGD-O2D-CED
24	7	313	CLA	O1D-CGD-O2D-CED
24	8	303	CLA	O1D-CGD-O2D-CED
24	8	308	CLA	O1D-CGD-O2D-CED
24	8	310	CLA	O1D-CGD-O2D-CED
24	S	603	CLA	O1D-CGD-O2D-CED
24	S	604	CLA	O1D-CGD-O2D-CED
24	Y	311	CLA	O1D-CGD-O2D-CED
24	b	603	CLA	O1D-CGD-O2D-CED
24	b	609	CLA	O1D-CGD-O2D-CED
24	n	610	CLA	O1D-CGD-O2D-CED
24	s	604	CLA	O1D-CGD-O2D-CED
24	s	608	CLA	O1D-CGD-O2D-CED
24	s	609	CLA	O1D-CGD-O2D-CED
24	C	503	CLA	O1D-CGD-O2D-CED
24	C	504	CLA	O1D-CGD-O2D-CED
24	C	510	CLA	O1D-CGD-O2D-CED
24	r	608	CLA	O1D-CGD-O2D-CED
24	r	611	CLA	O1D-CGD-O2D-CED
24	0	610	CLA	O1D-CGD-O2D-CED
24	AA	313	CLA	O1D-CGD-O2D-CED
24	AB	303	CLA	O1D-CGD-O2D-CED
24	AB	310	CLA	O1D-CGD-O2D-CED
24	v	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	v	606	CLA	O1D-CGD-O2D-CED
24	A6	603	CLA	O1D-CGD-O2D-CED
24	BB	311	CLA	O1D-CGD-O2D-CED
24	BB	312	CLA	O1D-CGD-O2D-CED
24	BE	609	CLA	O1D-CGD-O2D-CED
24	BQ	610	CLA	O1D-CGD-O2D-CED
24	BV	608	CLA	O1D-CGD-O2D-CED
24	1	504	CLA	O1D-CGD-O2D-CED
24	BF	507	CLA	O1D-CGD-O2D-CED
24	BU	611	CLA	O1D-CGD-O2D-CED
23	6	606	CHL	O1D-CGD-O2D-CED
23	7	307	CHL	O1D-CGD-O2D-CED
23	N	605	CHL	O1D-CGD-O2D-CED
23	N	606	CHL	O1D-CGD-O2D-CED
23	N	608	CHL	O1D-CGD-O2D-CED
23	Y	307	CHL	O1D-CGD-O2D-CED
23	Y	309	CHL	O1D-CGD-O2D-CED
23	n	606	CHL	O1D-CGD-O2D-CED
23	y	309	CHL	O1D-CGD-O2D-CED
23	0	606	CHL	O1D-CGD-O2D-CED
23	AA	307	CHL	O1D-CGD-O2D-CED
23	AA	309	CHL	O1D-CGD-O2D-CED
23	A2	605	CHL	O1D-CGD-O2D-CED
23	A2	606	CHL	O1D-CGD-O2D-CED
23	BB	307	CHL	O1D-CGD-O2D-CED
23	BB	309	CHL	O1D-CGD-O2D-CED
23	Ba	309	CHL	O1D-CGD-O2D-CED
24	5	611	CLA	O1D-CGD-O2D-CED
24	6	603	CLA	O1D-CGD-O2D-CED
24	6	612	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	O1D-CGD-O2D-CED
24	N	610	CLA	O1D-CGD-O2D-CED
24	N	614	CLA	O1D-CGD-O2D-CED
24	y	311	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	O1D-CGD-O2D-CED
24	c	511	CLA	O1D-CGD-O2D-CED
24	9	604	CLA	O1D-CGD-O2D-CED
24	9	611	CLA	O1D-CGD-O2D-CED
24	0	612	CLA	O1D-CGD-O2D-CED
24	AB	308	CLA	O1D-CGD-O2D-CED
24	v	602	CLA	O1D-CGD-O2D-CED
24	A2	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	BE	603	CLA	O1D-CGD-O2D-CED
24	BV	604	CLA	O1D-CGD-O2D-CED
24	Ba	311	CLA	O1D-CGD-O2D-CED
24	1	510	CLA	O1D-CGD-O2D-CED
24	N	610	CLA	CBA-CGA-O2A-C1
24	c	514	CLA	CBA-CGA-O2A-C1
24	r	610	CLA	CBA-CGA-O2A-C1
24	A2	610	CLA	CBA-CGA-O2A-C1
24	BF	514	CLA	CBA-CGA-O2A-C1
24	BU	610	CLA	CBA-CGA-O2A-C1
23	5	607	CHL	CBD-CGD-O2D-CED
23	6	609	CHL	CBD-CGD-O2D-CED
23	S	605	CHL	CBD-CGD-O2D-CED
23	S	607	CHL	CBD-CGD-O2D-CED
23	Y	306	CHL	CBD-CGD-O2D-CED
23	s	605	CHL	CBD-CGD-O2D-CED
23	s	607	CHL	CBD-CGD-O2D-CED
23	0	609	CHL	CBD-CGD-O2D-CED
23	A6	605	CHL	CBD-CGD-O2D-CED
23	BB	306	CHL	CBD-CGD-O2D-CED
23	BB	310	CHL	CBD-CGD-O2D-CED
23	BV	605	CHL	CBD-CGD-O2D-CED
24	7	304	CLA	CBD-CGD-O2D-CED
24	7	305	CLA	CBD-CGD-O2D-CED
24	B	607	CLA	CBD-CGD-O2D-CED
24	B	610	CLA	CBD-CGD-O2D-CED
24	B	611	CLA	CBD-CGD-O2D-CED
24	G	611	CLA	CBD-CGD-O2D-CED
24	G	612	CLA	CBD-CGD-O2D-CED
24	N	602	CLA	CBD-CGD-O2D-CED
24	S	612	CLA	CBD-CGD-O2D-CED
24	b	610	CLA	CBD-CGD-O2D-CED
24	b	611	CLA	CBD-CGD-O2D-CED
24	b	612	CLA	CBD-CGD-O2D-CED
24	g	612	CLA	CBD-CGD-O2D-CED
24	n	603	CLA	CBD-CGD-O2D-CED
24	y	303	CLA	CBD-CGD-O2D-CED
24	A	410	CLA	CBD-CGD-O2D-CED
24	a	406	CLA	CBD-CGD-O2D-CED
24	9	612	CLA	CBD-CGD-O2D-CED
24	AA	305	CLA	CBD-CGD-O2D-CED
24	v	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	v	611	CLA	CBD-CGD-O2D-CED
24	Au	611	CLA	CBD-CGD-O2D-CED
24	A2	602	CLA	CBD-CGD-O2D-CED
24	A6	612	CLA	CBD-CGD-O2D-CED
24	BE	611	CLA	CBD-CGD-O2D-CED
24	BE	612	CLA	CBD-CGD-O2D-CED
24	BJ	612	CLA	CBD-CGD-O2D-CED
24	BQ	603	CLA	CBD-CGD-O2D-CED
24	Ba	303	CLA	CBD-CGD-O2D-CED
24	R	409	CLA	CBD-CGD-O2D-CED
24	1	507	CLA	CBD-CGD-O2D-CED
24	BD	406	CLA	CBD-CGD-O2D-CED
24	BF	508	CLA	CBD-CGD-O2D-CED
38	A	409	PHO	CBD-CGD-O2D-CED
38	R	408	PHO	CBD-CGD-O2D-CED
23	7	310	CHL	O1A-CGA-O2A-C1
23	Y	309	CHL	O1A-CGA-O2A-C1
23	y	309	CHL	O1A-CGA-O2A-C1
23	BB	309	CHL	O1A-CGA-O2A-C1
23	Ba	309	CHL	O1A-CGA-O2A-C1
24	B	616	CLA	O1A-CGA-O2A-C1
24	D	402	CLA	O1A-CGA-O2A-C1
24	N	611	CLA	O1A-CGA-O2A-C1
24	d	402	CLA	O1A-CGA-O2A-C1
24	s	602	CLA	O1A-CGA-O2A-C1
24	C	506	CLA	O1A-CGA-O2A-C1
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	507	CLA	O1A-CGA-O2A-C1
24	v	616	CLA	O1A-CGA-O2A-C1
24	2	403	CLA	O1A-CGA-O2A-C1
24	A2	611	CLA	O1A-CGA-O2A-C1
24	BG	402	CLA	O1A-CGA-O2A-C1
24	1	506	CLA	O1A-CGA-O2A-C1
24	1	513	CLA	O1A-CGA-O2A-C1
24	BD	407	CLA	O1A-CGA-O2A-C1
24	BF	507	CLA	O1A-CGA-O2A-C1
34	a	401	DGD	O1A-C1A-O1G-C1G
34	BD	401	DGD	O1A-C1A-O1G-C1G
38	a	408	PHO	O1A-CGA-O2A-C1
38	R	407	PHO	O1A-CGA-O2A-C1
38	BD	408	PHO	O1A-CGA-O2A-C1
23	7	308	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	9	608	CHL	O1D-CGD-O2D-CED
23	AA	308	CHL	O1D-CGD-O2D-CED
23	A2	608	CHL	O1D-CGD-O2D-CED
23	BQ	606	CHL	O1D-CGD-O2D-CED
24	S	608	CLA	O1D-CGD-O2D-CED
24	0	603	CLA	O1D-CGD-O2D-CED
24	A2	610	CLA	O1D-CGD-O2D-CED
24	A6	608	CLA	O1D-CGD-O2D-CED
24	BF	511	CLA	O1D-CGD-O2D-CED
23	5	608	CHL	O1D-CGD-O2D-CED
23	AA	306	CHL	O1D-CGD-O2D-CED
24	5	614	CLA	O1D-CGD-O2D-CED
24	G	604	CLA	O1D-CGD-O2D-CED
24	b	617	CLA	O1D-CGD-O2D-CED
24	n	604	CLA	O1D-CGD-O2D-CED
24	s	611	CLA	O1D-CGD-O2D-CED
24	a	407	CLA	O1D-CGD-O2D-CED
24	0	604	CLA	O1D-CGD-O2D-CED
24	Au	604	CLA	O1D-CGD-O2D-CED
24	A6	604	CLA	O1D-CGD-O2D-CED
24	BE	617	CLA	O1D-CGD-O2D-CED
24	BQ	604	CLA	O1D-CGD-O2D-CED
24	BV	611	CLA	O1D-CGD-O2D-CED
24	1	506	CLA	O1D-CGD-O2D-CED
24	v	610	CLA	C4C-C3C-CAC-CBC
23	G	608	CHL	CBD-CGD-O2D-CED
24	b	608	CLA	CBD-CGD-O2D-CED
24	9	603	CLA	CBD-CGD-O2D-CED
24	BE	608	CLA	CBD-CGD-O2D-CED
24	BE	610	CLA	CBD-CGD-O2D-CED
23	7	306	CHL	O1D-CGD-O2D-CED
23	Ba	310	CHL	O1D-CGD-O2D-CED
24	g	604	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	O1D-CGD-O2D-CED
24	v	609	CLA	O1D-CGD-O2D-CED
24	BJ	604	CLA	O1D-CGD-O2D-CED
27	C	520	LHG	O9-C7-O7-C5
27	1	520	LHG	O9-C7-O7-C5
32	D	406	SQD	O49-C7-O47-C45
32	L	103	SQD	O49-C7-O47-C45
32	d	406	SQD	O49-C7-O47-C45
32	l	101	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
32	2	408	SQD	O49-C7-O47-C45
32	A1	101	SQD	O49-C7-O47-C45
32	BG	406	SQD	O49-C7-O47-C45
32	BO	101	SQD	O49-C7-O47-C45
34	C	518	DGD	O1B-C1B-O2G-C2G
34	1	518	DGD	O1B-C1B-O2G-C2G
23	AA	310	CHL	O1A-CGA-O2A-C1
24	y	315	CLA	O1A-CGA-O2A-C1
38	A	408	PHO	O1A-CGA-O2A-C1
24	B	610	CLA	C4C-C3C-CAC-CBC
24	9	614	CLA	O1D-CGD-O2D-CED
24	BD	407	CLA	O1D-CGD-O2D-CED
24	6	613	CLA	C3-C5-C6-C7
24	B	605	CLA	C3-C5-C6-C7
24	B	607	CLA	C3-C5-C6-C7
24	B	616	CLA	C3-C5-C6-C7
24	G	612	CLA	C3-C5-C6-C7
24	N	610	CLA	C3-C5-C6-C7
24	S	610	CLA	C3-C5-C6-C7
24	b	606	CLA	C3-C5-C6-C7
24	b	615	CLA	C3-C5-C6-C7
24	n	610	CLA	C3-C5-C6-C7
24	s	610	CLA	C3-C5-C6-C7
24	C	504	CLA	C3-C5-C6-C7
24	c	506	CLA	C3-C5-C6-C7
24	r	603	CLA	C3-C5-C6-C7
24	0	613	CLA	C3-C5-C6-C7
24	v	607	CLA	C3-C5-C6-C7
24	v	616	CLA	C3-C5-C6-C7
24	Au	612	CLA	C3-C5-C6-C7
24	A2	610	CLA	C3-C5-C6-C7
24	A6	610	CLA	C3-C5-C6-C7
24	BE	606	CLA	C3-C5-C6-C7
24	BE	615	CLA	C3-C5-C6-C7
24	BQ	610	CLA	C3-C5-C6-C7
24	BV	610	CLA	C3-C5-C6-C7
24	1	504	CLA	C3-C5-C6-C7
24	BF	506	CLA	C3-C5-C6-C7
24	BU	603	CLA	C3-C5-C6-C7
38	A	408	PHO	C3-C5-C6-C7
38	a	408	PHO	C3-C5-C6-C7
38	R	407	PHO	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
38	BD	408	PHO	C3-C5-C6-C7
23	6	609	CHL	CBA-CGA-O2A-C1
23	y	310	CHL	CBA-CGA-O2A-C1
23	0	609	CHL	CBA-CGA-O2A-C1
23	Ba	310	CHL	CBA-CGA-O2A-C1
24	B	616	CLA	CBA-CGA-O2A-C1
24	S	602	CLA	CBA-CGA-O2A-C1
24	S	613	CLA	CBA-CGA-O2A-C1
24	b	617	CLA	CBA-CGA-O2A-C1
24	s	602	CLA	CBA-CGA-O2A-C1
24	A	407	CLA	CBA-CGA-O2A-C1
24	a	407	CLA	CBA-CGA-O2A-C1
24	a	410	CLA	CBA-CGA-O2A-C1
24	A6	602	CLA	CBA-CGA-O2A-C1
24	A6	613	CLA	CBA-CGA-O2A-C1
24	BE	617	CLA	CBA-CGA-O2A-C1
24	R	406	CLA	CBA-CGA-O2A-C1
24	R	409	CLA	CBA-CGA-O2A-C1
24	BD	407	CLA	CBA-CGA-O2A-C1
24	BD	410	CLA	CBA-CGA-O2A-C1
30	c	501	LMG	C29-C28-O8-C9
30	BF	501	LMG	C29-C28-O8-C9
34	a	401	DGD	C2A-C1A-O1G-C1G
34	BD	401	DGD	C2A-C1A-O1G-C1G
23	G	606	CHL	O1D-CGD-O2D-CED
23	Au	606	CHL	O1D-CGD-O2D-CED
24	B	616	CLA	O1D-CGD-O2D-CED
24	c	503	CLA	O1D-CGD-O2D-CED
24	c	504	CLA	O1D-CGD-O2D-CED
24	v	616	CLA	O1D-CGD-O2D-CED
24	BV	609	CLA	O1D-CGD-O2D-CED
24	BF	504	CLA	O1D-CGD-O2D-CED
23	Au	608	CHL	CBD-CGD-O2D-CED
24	N	603	CLA	CBD-CGD-O2D-CED
24	g	603	CLA	CBD-CGD-O2D-CED
24	B	610	CLA	C2C-C3C-CAC-CBC
24	v	610	CLA	C2C-C3C-CAC-CBC
24	b	609	CLA	O1A-CGA-O2A-C1
23	5	601	CHL	C2C-C3C-CAC-CBC
23	5	607	CHL	C3-C5-C6-C7
23	6	601	CHL	C3-C5-C6-C7
23	9	607	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	0	601	CHL	C3-C5-C6-C7
23	Ba	302	CHL	C4-C3-C5-C6
24	B	607	CLA	C4-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	v	607	CLA	C4-C3-C5-C6
23	n	601	CHL	C2-C3-C5-C6
23	BQ	601	CHL	C2-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	v	605	CLA	C2-C3-C5-C6
24	Au	611	CLA	C2-C3-C5-C6
24	1	508	CLA	C2-C3-C5-C6
23	7	310	CHL	CBD-CGD-O2D-CED
23	g	607	CHL	CBD-CGD-O2D-CED
23	y	308	CHL	CBD-CGD-O2D-CED
23	AA	310	CHL	CBD-CGD-O2D-CED
23	Ba	308	CHL	CBD-CGD-O2D-CED
24	BJ	603	CLA	CBD-CGD-O2D-CED
23	6	606	CHL	C2A-CAA-CBA-CGA
23	6	609	CHL	C2A-CAA-CBA-CGA
23	7	306	CHL	C2A-CAA-CBA-CGA
23	7	308	CHL	C2A-CAA-CBA-CGA
23	7	310	CHL	C2A-CAA-CBA-CGA
23	G	607	CHL	C2A-CAA-CBA-CGA
23	G	608	CHL	C2A-CAA-CBA-CGA
23	N	605	CHL	C2A-CAA-CBA-CGA
23	Y	308	CHL	C2A-CAA-CBA-CGA
23	Y	309	CHL	C2A-CAA-CBA-CGA
23	g	607	CHL	C2A-CAA-CBA-CGA
23	g	608	CHL	C2A-CAA-CBA-CGA
23	s	607	CHL	C2A-CAA-CBA-CGA
23	y	308	CHL	C2A-CAA-CBA-CGA
23	r	607	CHL	C2A-CAA-CBA-CGA
23	9	608	CHL	C2A-CAA-CBA-CGA
23	0	606	CHL	C2A-CAA-CBA-CGA
23	AA	306	CHL	C2A-CAA-CBA-CGA
23	AA	308	CHL	C2A-CAA-CBA-CGA
23	AA	310	CHL	C2A-CAA-CBA-CGA
23	Au	607	CHL	C2A-CAA-CBA-CGA
23	Au	608	CHL	C2A-CAA-CBA-CGA
23	A2	605	CHL	C2A-CAA-CBA-CGA
23	BB	308	CHL	C2A-CAA-CBA-CGA
23	BB	309	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	BJ	607	CHL	C2A-CAA-CBA-CGA
23	BJ	608	CHL	C2A-CAA-CBA-CGA
23	BV	607	CHL	C2A-CAA-CBA-CGA
23	Ba	308	CHL	C2A-CAA-CBA-CGA
23	BU	607	CHL	C2A-CAA-CBA-CGA
24	5	611	CLA	C2A-CAA-CBA-CGA
24	5	613	CLA	C2A-CAA-CBA-CGA
24	6	611	CLA	C2A-CAA-CBA-CGA
24	7	312	CLA	C2A-CAA-CBA-CGA
24	8	309	CLA	C2A-CAA-CBA-CGA
24	B	604	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C2A-CAA-CBA-CGA
24	I	102	CLA	C2A-CAA-CBA-CGA
24	b	605	CLA	C2A-CAA-CBA-CGA
24	b	615	CLA	C2A-CAA-CBA-CGA
24	C	505	CLA	C2A-CAA-CBA-CGA
24	C	511	CLA	C2A-CAA-CBA-CGA
24	a	405	CLA	C2A-CAA-CBA-CGA
24	a	406	CLA	C2A-CAA-CBA-CGA
24	c	505	CLA	C2A-CAA-CBA-CGA
24	r	610	CLA	C2A-CAA-CBA-CGA
24	9	611	CLA	C2A-CAA-CBA-CGA
24	9	613	CLA	C2A-CAA-CBA-CGA
24	0	611	CLA	C2A-CAA-CBA-CGA
24	AA	312	CLA	C2A-CAA-CBA-CGA
24	AA	315	CLA	C2A-CAA-CBA-CGA
24	AB	309	CLA	C2A-CAA-CBA-CGA
24	v	604	CLA	C2A-CAA-CBA-CGA
24	v	614	CLA	C2A-CAA-CBA-CGA
24	Aw	102	CLA	C2A-CAA-CBA-CGA
24	BE	605	CLA	C2A-CAA-CBA-CGA
24	BE	615	CLA	C2A-CAA-CBA-CGA
24	BQ	611	CLA	C2A-CAA-CBA-CGA
24	BV	602	CLA	C2A-CAA-CBA-CGA
24	Ba	305	CLA	C2A-CAA-CBA-CGA
24	1	505	CLA	C2A-CAA-CBA-CGA
24	BD	405	CLA	C2A-CAA-CBA-CGA
24	BD	406	CLA	C2A-CAA-CBA-CGA
24	BF	505	CLA	C2A-CAA-CBA-CGA
24	BU	610	CLA	C2A-CAA-CBA-CGA
38	A	409	PHO	C2A-CAA-CBA-CGA
38	R	408	PHO	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	Ba	315	CLA	O1A-CGA-O2A-C1
23	9	601	CHL	C2C-C3C-CAC-CBC
24	b	608	CLA	C3-C5-C6-C7
24	g	612	CLA	C3-C5-C6-C7
24	y	314	CLA	C3-C5-C6-C7
24	C	512	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
24	v	605	CLA	C3-C5-C6-C7
24	BE	608	CLA	C3-C5-C6-C7
24	BJ	612	CLA	C3-C5-C6-C7
24	Ba	314	CLA	C3-C5-C6-C7
24	1	512	CLA	C3-C5-C6-C7
24	BF	513	CLA	C3-C5-C6-C7
23	5	609	CHL	CBA-CGA-O2A-C1
23	7	310	CHL	CBA-CGA-O2A-C1
23	N	601	CHL	CBA-CGA-O2A-C1
23	N	609	CHL	CBA-CGA-O2A-C1
23	Y	309	CHL	CBA-CGA-O2A-C1
23	g	609	CHL	CBA-CGA-O2A-C1
23	n	609	CHL	CBA-CGA-O2A-C1
23	y	309	CHL	CBA-CGA-O2A-C1
23	AA	310	CHL	CBA-CGA-O2A-C1
23	A2	601	CHL	CBA-CGA-O2A-C1
23	BB	309	CHL	CBA-CGA-O2A-C1
23	BJ	609	CHL	CBA-CGA-O2A-C1
23	BQ	601	CHL	CBA-CGA-O2A-C1
23	BQ	609	CHL	CBA-CGA-O2A-C1
23	Ba	309	CHL	CBA-CGA-O2A-C1
24	B	610	CLA	CBA-CGA-O2A-C1
24	B	614	CLA	CBA-CGA-O2A-C1
24	D	402	CLA	CBA-CGA-O2A-C1
24	N	611	CLA	CBA-CGA-O2A-C1
24	Y	315	CLA	CBA-CGA-O2A-C1
24	b	609	CLA	CBA-CGA-O2A-C1
24	d	402	CLA	CBA-CGA-O2A-C1
24	n	611	CLA	CBA-CGA-O2A-C1
24	s	613	CLA	CBA-CGA-O2A-C1
24	y	315	CLA	CBA-CGA-O2A-C1
24	A	410	CLA	CBA-CGA-O2A-C1
24	C	502	CLA	CBA-CGA-O2A-C1
24	C	506	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	c	502	CLA	CBA-CGA-O2A-C1
24	c	507	CLA	CBA-CGA-O2A-C1
24	v	610	CLA	CBA-CGA-O2A-C1
24	v	614	CLA	CBA-CGA-O2A-C1
24	v	616	CLA	CBA-CGA-O2A-C1
24	2	403	CLA	CBA-CGA-O2A-C1
24	A2	611	CLA	CBA-CGA-O2A-C1
24	BB	315	CLA	CBA-CGA-O2A-C1
24	BG	402	CLA	CBA-CGA-O2A-C1
24	BQ	611	CLA	CBA-CGA-O2A-C1
24	BV	613	CLA	CBA-CGA-O2A-C1
24	1	502	CLA	CBA-CGA-O2A-C1
24	1	506	CLA	CBA-CGA-O2A-C1
24	1	513	CLA	CBA-CGA-O2A-C1
24	BF	502	CLA	CBA-CGA-O2A-C1
24	BF	507	CLA	CBA-CGA-O2A-C1
30	C	501	LMG	C29-C28-O8-C9
30	1	501	LMG	C29-C28-O8-C9
34	A	402	DGD	C2A-C1A-O1G-C1G
34	R	401	DGD	C2A-C1A-O1G-C1G
38	A	408	PHO	CBA-CGA-O2A-C1
38	a	408	PHO	CBA-CGA-O2A-C1
38	R	407	PHO	CBA-CGA-O2A-C1
38	BD	408	PHO	CBA-CGA-O2A-C1
23	g	606	CHL	O1D-CGD-O2D-CED
23	BJ	606	CHL	O1D-CGD-O2D-CED
24	B	609	CLA	O1D-CGD-O2D-CED
24	y	312	CLA	O1D-CGD-O2D-CED
24	BF	503	CLA	O1D-CGD-O2D-CED
23	BQ	607	CHL	CBD-CGD-O2D-CED
23	BU	607	CHL	CBD-CGD-O2D-CED
24	6	613	CLA	CBD-CGD-O2D-CED
24	D	401	CLA	CBD-CGD-O2D-CED
24	Au	612	CLA	CBD-CGD-O2D-CED
23	BJ	609	CHL	C2C-C3C-CAC-CBC
23	n	605	CHL	O1D-CGD-O2D-CED
23	A6	607	CHL	O1D-CGD-O2D-CED
24	6	604	CLA	O1D-CGD-O2D-CED
24	7	303	CLA	O1D-CGD-O2D-CED
24	8	302	CLA	O1D-CGD-O2D-CED
24	B	614	CLA	O1D-CGD-O2D-CED
24	S	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	Y	305	CLA	O1D-CGD-O2D-CED
24	c	508	CLA	O1D-CGD-O2D-CED
24	AA	303	CLA	O1D-CGD-O2D-CED
24	AB	302	CLA	O1D-CGD-O2D-CED
24	v	614	CLA	O1D-CGD-O2D-CED
24	A6	611	CLA	O1D-CGD-O2D-CED
24	BB	305	CLA	O1D-CGD-O2D-CED
24	Ba	312	CLA	O1D-CGD-O2D-CED
27	c	519	LHG	O9-C7-O7-C5
27	BF	520	LHG	O9-C7-O7-C5
34	c	516	DGD	C4E-C5E-C6E-O5E
34	1	516	DGD	C4E-C5E-C6E-O5E
34	BF	517	DGD	C4E-C5E-C6E-O5E
23	g	609	CHL	O1A-CGA-O2A-C1
23	n	609	CHL	O1A-CGA-O2A-C1
23	y	310	CHL	O1A-CGA-O2A-C1
23	BJ	609	CHL	O1A-CGA-O2A-C1
23	BQ	609	CHL	O1A-CGA-O2A-C1
23	Ba	310	CHL	O1A-CGA-O2A-C1
24	B	608	CLA	O1A-CGA-O2A-C1
24	S	613	CLA	O1A-CGA-O2A-C1
24	Y	315	CLA	O1A-CGA-O2A-C1
24	g	614	CLA	O1A-CGA-O2A-C1
24	n	611	CLA	O1A-CGA-O2A-C1
24	v	608	CLA	O1A-CGA-O2A-C1
24	A6	602	CLA	O1A-CGA-O2A-C1
24	A6	613	CLA	O1A-CGA-O2A-C1
24	BB	315	CLA	O1A-CGA-O2A-C1
24	BE	609	CLA	O1A-CGA-O2A-C1
24	BJ	614	CLA	O1A-CGA-O2A-C1
24	BQ	611	CLA	O1A-CGA-O2A-C1
24	BV	602	CLA	O1A-CGA-O2A-C1
34	A	402	DGD	O1A-C1A-O1G-C1G
34	R	401	DGD	O1A-C1A-O1G-C1G
23	g	609	CHL	C2C-C3C-CAC-CBC
23	BQ	605	CHL	O1D-CGD-O2D-CED
26	G	617	NEX	C9-C10-C11-C12
26	Y	318	NEX	C13-C14-C15-C35
26	r	617	NEX	C13-C14-C15-C35
26	Au	617	NEX	C9-C10-C11-C12
26	BB	320	NEX	C13-C14-C15-C35
30	I	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
34	C	516	DGD	C4E-C5E-C6E-O5E
23	6	601	CHL	CBD-CGD-O2D-CED
23	G	605	CHL	CBD-CGD-O2D-CED
23	n	607	CHL	CBD-CGD-O2D-CED
23	0	601	CHL	CBD-CGD-O2D-CED
23	Au	605	CHL	CBD-CGD-O2D-CED
23	BB	302	CHL	CBD-CGD-O2D-CED
23	BJ	607	CHL	CBD-CGD-O2D-CED
24	B	615	CLA	CBD-CGD-O2D-CED
24	Y	303	CLA	CBD-CGD-O2D-CED
24	a	410	CLA	CBD-CGD-O2D-CED
24	v	610	CLA	CBD-CGD-O2D-CED
24	v	615	CLA	CBD-CGD-O2D-CED
24	2	402	CLA	CBD-CGD-O2D-CED
24	1	511	CLA	CBD-CGD-O2D-CED
24	BD	410	CLA	CBD-CGD-O2D-CED
38	a	409	PHO	CBD-CGD-O2D-CED
38	BD	409	PHO	CBD-CGD-O2D-CED
23	BV	607	CHL	O1D-CGD-O2D-CED
27	5	618	LHG	O2-C2-C3-O3
27	N	618	LHG	O2-C2-C3-O3
27	n	618	LHG	O2-C2-C3-O3
27	C	520	LHG	O2-C2-C3-O3
27	c	519	LHG	O2-C2-C3-O3
27	9	618	LHG	O2-C2-C3-O3
27	A2	618	LHG	O2-C2-C3-O3
27	BQ	618	LHG	O2-C2-C3-O3
27	1	520	LHG	O2-C2-C3-O3
27	BF	520	LHG	O2-C2-C3-O3
24	y	303	CLA	C3-C5-C6-C7
24	y	311	CLA	C3-C5-C6-C7
24	BQ	602	CLA	C3-C5-C6-C7
24	Ba	303	CLA	C3-C5-C6-C7
23	n	601	CHL	CBA-CGA-O2A-C1
23	9	609	CHL	CBA-CGA-O2A-C1
23	0	601	CHL	CBA-CGA-O2A-C1
23	A2	609	CHL	CBA-CGA-O2A-C1
24	6	603	CLA	CBA-CGA-O2A-C1
24	B	604	CLA	CBA-CGA-O2A-C1
24	b	611	CLA	CBA-CGA-O2A-C1
24	b	615	CLA	CBA-CGA-O2A-C1
24	s	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	CBA-CGA-O2A-C1
24	C	511	CLA	CBA-CGA-O2A-C1
24	0	603	CLA	CBA-CGA-O2A-C1
24	v	604	CLA	CBA-CGA-O2A-C1
24	BB	311	CLA	CBA-CGA-O2A-C1
24	BE	611	CLA	CBA-CGA-O2A-C1
24	BE	615	CLA	CBA-CGA-O2A-C1
24	BV	604	CLA	CBA-CGA-O2A-C1
24	Ba	315	CLA	CBA-CGA-O2A-C1
24	1	510	CLA	CBA-CGA-O2A-C1
34	c	517	DGD	C2A-C1A-O1G-C1G
34	BF	518	DGD	C2A-C1A-O1G-C1G
24	S	602	CLA	O1A-CGA-O2A-C1
24	A	410	CLA	O1A-CGA-O2A-C1
24	C	502	CLA	O1A-CGA-O2A-C1
24	a	410	CLA	O1A-CGA-O2A-C1
24	R	409	CLA	O1A-CGA-O2A-C1
24	BD	410	CLA	O1A-CGA-O2A-C1
24	G	603	CLA	O1D-CGD-O2D-CED
27	C	520	LHG	C8-C7-O7-C5
27	c	519	LHG	C8-C7-O7-C5
27	1	520	LHG	C8-C7-O7-C5
27	BF	520	LHG	C8-C7-O7-C5
23	Y	302	CHL	CBD-CGD-O2D-CED
23	y	302	CHL	CBD-CGD-O2D-CED
23	r	605	CHL	CBD-CGD-O2D-CED
23	r	607	CHL	CBD-CGD-O2D-CED
23	9	607	CHL	CBD-CGD-O2D-CED
23	Au	601	CHL	CBD-CGD-O2D-CED
23	Ba	302	CHL	CBD-CGD-O2D-CED
23	BU	605	CHL	CBD-CGD-O2D-CED
24	g	602	CLA	CBD-CGD-O2D-CED
24	y	313	CLA	CBD-CGD-O2D-CED
24	0	613	CLA	CBD-CGD-O2D-CED
24	A2	603	CLA	CBD-CGD-O2D-CED
24	BV	612	CLA	CBD-CGD-O2D-CED
30	Aw	101	LMG	O6-C5-C6-O5
23	A2	609	CHL	O1A-CGA-O2A-C1
23	BQ	601	CHL	O1A-CGA-O2A-C1
24	v	610	CLA	O1A-CGA-O2A-C1
24	BE	615	CLA	O1A-CGA-O2A-C1
24	1	502	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	D	404	LHG	C28-C29-C30-C31
34	H	102	DGD	O6D-C5D-C6D-O5D
26	BB	318	NEX	C14-C15-C35-C34
24	b	614	CLA	C3-C5-C6-C7
24	BE	614	CLA	C3-C5-C6-C7
23	G	609	CHL	CBA-CGA-O2A-C1
24	7	304	CLA	CBA-CGA-O2A-C1
24	B	608	CLA	CBA-CGA-O2A-C1
24	b	605	CLA	CBA-CGA-O2A-C1
24	g	614	CLA	CBA-CGA-O2A-C1
24	AA	304	CLA	CBA-CGA-O2A-C1
24	v	608	CLA	CBA-CGA-O2A-C1
24	BE	605	CLA	CBA-CGA-O2A-C1
24	BE	609	CLA	CBA-CGA-O2A-C1
24	BJ	614	CLA	CBA-CGA-O2A-C1
24	BV	602	CLA	CBA-CGA-O2A-C1
24	5	603	CLA	O1D-CGD-O2D-CED
24	G	611	CLA	O1D-CGD-O2D-CED
24	N	604	CLA	O1D-CGD-O2D-CED
23	5	609	CHL	O1A-CGA-O2A-C1
23	N	609	CHL	O1A-CGA-O2A-C1
23	n	601	CHL	O1A-CGA-O2A-C1
24	6	603	CLA	O1A-CGA-O2A-C1
24	B	610	CLA	O1A-CGA-O2A-C1
24	B	614	CLA	O1A-CGA-O2A-C1
24	b	615	CLA	O1A-CGA-O2A-C1
24	s	604	CLA	O1A-CGA-O2A-C1
24	s	613	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
24	c	502	CLA	O1A-CGA-O2A-C1
24	0	603	CLA	O1A-CGA-O2A-C1
24	v	614	CLA	O1A-CGA-O2A-C1
24	BV	613	CLA	O1A-CGA-O2A-C1
27	c	519	LHG	O10-C23-O8-C6
27	BF	520	LHG	O10-C23-O8-C6
33	BI	102	HEM	C3D-CAD-CBD-CGD
23	r	607	CHL	C3-C5-C6-C7
23	BU	607	CHL	C3-C5-C6-C7
27	2	406	LHG	C28-C29-C30-C31
32	R	411	SQD	C17-C18-C19-C20
34	C	516	DGD	O6E-C5E-C6E-O5E
23	N	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	A2	601	CHL	C4-C3-C5-C6
24	6	613	CLA	C4-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	613	CLA	C4-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	b	604	CLA	C4-C3-C5-C6
24	b	606	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
24	v	602	CLA	C4-C3-C5-C6
24	v	603	CLA	C4-C3-C5-C6
24	v	613	CLA	C4-C3-C5-C6
24	v	615	CLA	C4-C3-C5-C6
24	BE	603	CLA	C4-C3-C5-C6
24	BE	604	CLA	C4-C3-C5-C6
24	BE	606	CLA	C4-C3-C5-C6
24	BE	614	CLA	C4-C3-C5-C6
23	N	601	CHL	C2-C3-C5-C6
23	0	601	CHL	C2-C3-C5-C6
23	A2	601	CHL	C2-C3-C5-C6
24	B	603	CLA	C2-C3-C5-C6
24	B	613	CLA	C2-C3-C5-C6
24	B	615	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	b	604	CLA	C2-C3-C5-C6
24	b	606	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
24	v	602	CLA	C2-C3-C5-C6
24	v	603	CLA	C2-C3-C5-C6
24	v	613	CLA	C2-C3-C5-C6
24	v	615	CLA	C2-C3-C5-C6
24	BE	603	CLA	C2-C3-C5-C6
24	BE	604	CLA	C2-C3-C5-C6
24	BE	606	CLA	C2-C3-C5-C6
24	BE	614	CLA	C2-C3-C5-C6
34	Av	102	DGD	O6D-C5D-C6D-O5D
23	N	607	CHL	C2A-CAA-CBA-CGA
23	g	609	CHL	C2A-CAA-CBA-CGA
23	n	605	CHL	C2A-CAA-CBA-CGA
23	n	607	CHL	C2A-CAA-CBA-CGA
23	0	609	CHL	C2A-CAA-CBA-CGA
23	A2	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	BQ	605	CHL	C2A-CAA-CBA-CGA
24	S	602	CLA	C2A-CAA-CBA-CGA
24	Y	311	CLA	C2A-CAA-CBA-CGA
24	n	611	CLA	C2A-CAA-CBA-CGA
24	A	405	CLA	C2A-CAA-CBA-CGA
24	C	502	CLA	C2A-CAA-CBA-CGA
24	A6	602	CLA	C2A-CAA-CBA-CGA
24	BB	311	CLA	C2A-CAA-CBA-CGA
24	R	404	CLA	C2A-CAA-CBA-CGA
24	1	502	CLA	C2A-CAA-CBA-CGA
24	1	508	CLA	C2A-CAA-CBA-CGA
24	C	507	CLA	O1D-CGD-O2D-CED
24	A2	604	CLA	O1D-CGD-O2D-CED
27	N	618	LHG	C28-C29-C30-C31
27	A2	618	LHG	C28-C29-C30-C31
34	c	516	DGD	O6E-C5E-C6E-O5E
34	1	516	DGD	O6E-C5E-C6E-O5E
34	BF	517	DGD	O6E-C5E-C6E-O5E
23	G	609	CHL	O1A-CGA-O2A-C1
23	N	601	CHL	O1A-CGA-O2A-C1
23	9	609	CHL	O1A-CGA-O2A-C1
23	0	601	CHL	O1A-CGA-O2A-C1
23	A2	601	CHL	O1A-CGA-O2A-C1
24	B	604	CLA	O1A-CGA-O2A-C1
24	b	611	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	O1A-CGA-O2A-C1
24	AA	304	CLA	O1A-CGA-O2A-C1
24	v	604	CLA	O1A-CGA-O2A-C1
24	BB	311	CLA	O1A-CGA-O2A-C1
24	BE	611	CLA	O1A-CGA-O2A-C1
24	BV	604	CLA	O1A-CGA-O2A-C1
24	BF	502	CLA	O1A-CGA-O2A-C1
32	D	406	SQD	O5-C1-O6-C44
32	L	101	SQD	O5-C1-O6-C44
32	A	413	SQD	O5-C1-O6-C44
32	R	411	SQD	O5-C1-O6-C44
23	S	607	CHL	O1D-CGD-O2D-CED
31	D	403	PL9	C39-C41-C42-C43
31	d	403	PL9	C39-C41-C42-C43
31	2	404	PL9	C39-C41-C42-C43
31	BG	403	PL9	C39-C41-C42-C43
23	g	607	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
32	A	413	SQD	C17-C18-C19-C20
24	n	602	CLA	C3-C5-C6-C7
23	6	607	CHL	CBA-CGA-O2A-C1
23	g	601	CHL	CBA-CGA-O2A-C1
23	0	607	CHL	CBA-CGA-O2A-C1
23	BJ	601	CHL	CBA-CGA-O2A-C1
24	5	613	CLA	CBA-CGA-O2A-C1
24	G	614	CLA	CBA-CGA-O2A-C1
24	Y	311	CLA	CBA-CGA-O2A-C1
24	b	603	CLA	CBA-CGA-O2A-C1
24	d	401	CLA	CBA-CGA-O2A-C1
24	n	614	CLA	CBA-CGA-O2A-C1
24	r	609	CLA	CBA-CGA-O2A-C1
24	9	602	CLA	CBA-CGA-O2A-C1
24	v	615	CLA	CBA-CGA-O2A-C1
24	Au	614	CLA	CBA-CGA-O2A-C1
24	BQ	614	CLA	CBA-CGA-O2A-C1
24	1	511	CLA	CBA-CGA-O2A-C1
24	BU	609	CLA	CBA-CGA-O2A-C1
32	A	413	SQD	C24-C23-O48-C46
32	R	411	SQD	C24-C23-O48-C46
34	C	517	DGD	C2A-C1A-O1G-C1G
23	Ba	308	CHL	C2C-C3C-CAC-CBC
24	6	614	CLA	CBD-CGD-O2D-CED
24	Ba	313	CLA	CBD-CGD-O2D-CED
24	Au	603	CLA	O1D-CGD-O2D-CED
34	a	413	DGD	O6E-C5E-C6E-O5E
27	BQ	618	LHG	C28-C29-C30-C31
23	Y	310	CHL	O1D-CGD-O2D-CED
23	y	306	CHL	O1D-CGD-O2D-CED
24	5	612	CLA	O1D-CGD-O2D-CED
24	AA	304	CLA	O1D-CGD-O2D-CED
24	7	304	CLA	O1A-CGA-O2A-C1
24	G	614	CLA	O1A-CGA-O2A-C1
24	n	614	CLA	O1A-CGA-O2A-C1
24	Au	614	CLA	O1A-CGA-O2A-C1
24	BE	605	CLA	O1A-CGA-O2A-C1
24	BQ	614	CLA	O1A-CGA-O2A-C1
24	1	510	CLA	O1A-CGA-O2A-C1
27	n	618	LHG	C28-C29-C30-C31
23	6	609	CHL	O1D-CGD-O2D-CED
23	s	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	0	609	CHL	O1D-CGD-O2D-CED
23	Ba	306	CHL	O1D-CGD-O2D-CED
24	7	304	CLA	O1D-CGD-O2D-CED
24	S	612	CLA	O1D-CGD-O2D-CED
24	9	612	CLA	O1D-CGD-O2D-CED
24	A6	612	CLA	O1D-CGD-O2D-CED
24	1	507	CLA	O1D-CGD-O2D-CED
24	BJ	602	CLA	CBD-CGD-O2D-CED
24	R	406	CLA	CBD-CGD-O2D-CED
27	b	624	LHG	C1-C2-C3-O3
27	BE	624	LHG	C1-C2-C3-O3
34	a	413	DGD	O1B-C1B-O2G-C2G
34	BD	413	DGD	O1B-C1B-O2G-C2G
23	Y	310	CHL	O1A-CGA-O2A-C1
24	5	613	CLA	O1A-CGA-O2A-C1
24	Y	311	CLA	O1A-CGA-O2A-C1
24	b	605	CLA	O1A-CGA-O2A-C1
24	d	401	CLA	O1A-CGA-O2A-C1
24	1	511	CLA	O1A-CGA-O2A-C1
24	5	603	CLA	C3-C5-C6-C7
24	b	617	CLA	C3-C5-C6-C7
24	g	613	CLA	C3-C5-C6-C7
24	c	504	CLA	C3-C5-C6-C7
24	9	603	CLA	C3-C5-C6-C7
24	BE	617	CLA	C3-C5-C6-C7
24	BJ	613	CLA	C3-C5-C6-C7
24	1	507	CLA	C3-C5-C6-C7
23	Y	306	CHL	O1D-CGD-O2D-CED
23	BB	306	CHL	O1D-CGD-O2D-CED
24	a	406	CLA	O1D-CGD-O2D-CED
24	Au	611	CLA	O1D-CGD-O2D-CED
38	R	408	PHO	O1D-CGD-O2D-CED
23	6	601	CHL	CBA-CGA-O2A-C1
23	G	601	CHL	CBA-CGA-O2A-C1
23	Y	302	CHL	CBA-CGA-O2A-C1
23	Y	310	CHL	CBA-CGA-O2A-C1
23	y	302	CHL	CBA-CGA-O2A-C1
23	r	607	CHL	CBA-CGA-O2A-C1
23	Au	601	CHL	CBA-CGA-O2A-C1
23	Au	609	CHL	CBA-CGA-O2A-C1
23	BB	302	CHL	CBA-CGA-O2A-C1
23	BB	310	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	Ba	302	CHL	CBA-CGA-O2A-C1
23	BU	607	CHL	CBA-CGA-O2A-C1
24	5	602	CLA	CBA-CGA-O2A-C1
24	6	602	CLA	CBA-CGA-O2A-C1
24	B	601	CLA	CBA-CGA-O2A-C1
24	B	606	CLA	CBA-CGA-O2A-C1
24	B	612	CLA	CBA-CGA-O2A-C1
24	B	615	CLA	CBA-CGA-O2A-C1
24	D	401	CLA	CBA-CGA-O2A-C1
24	G	603	CLA	CBA-CGA-O2A-C1
24	G	610	CLA	CBA-CGA-O2A-C1
24	I	102	CLA	CBA-CGA-O2A-C1
24	N	603	CLA	CBA-CGA-O2A-C1
24	N	614	CLA	CBA-CGA-O2A-C1
24	S	604	CLA	CBA-CGA-O2A-C1
24	S	612	CLA	CBA-CGA-O2A-C1
24	b	602	CLA	CBA-CGA-O2A-C1
24	b	607	CLA	CBA-CGA-O2A-C1
24	b	608	CLA	CBA-CGA-O2A-C1
24	b	613	CLA	CBA-CGA-O2A-C1
24	g	603	CLA	CBA-CGA-O2A-C1
24	g	611	CLA	CBA-CGA-O2A-C1
24	n	603	CLA	CBA-CGA-O2A-C1
24	n	613	CLA	CBA-CGA-O2A-C1
24	y	303	CLA	CBA-CGA-O2A-C1
24	c	511	CLA	CBA-CGA-O2A-C1
24	r	608	CLA	CBA-CGA-O2A-C1
24	9	613	CLA	CBA-CGA-O2A-C1
24	0	602	CLA	CBA-CGA-O2A-C1
24	v	601	CLA	CBA-CGA-O2A-C1
24	v	606	CLA	CBA-CGA-O2A-C1
24	v	612	CLA	CBA-CGA-O2A-C1
24	2	402	CLA	CBA-CGA-O2A-C1
24	Au	603	CLA	CBA-CGA-O2A-C1
24	Au	610	CLA	CBA-CGA-O2A-C1
24	Aw	102	CLA	CBA-CGA-O2A-C1
24	A2	603	CLA	CBA-CGA-O2A-C1
24	A2	614	CLA	CBA-CGA-O2A-C1
24	A6	604	CLA	CBA-CGA-O2A-C1
24	A6	612	CLA	CBA-CGA-O2A-C1
24	BE	602	CLA	CBA-CGA-O2A-C1
24	BE	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	BE	607	CLA	CBA-CGA-O2A-C1
24	BE	608	CLA	CBA-CGA-O2A-C1
24	BE	613	CLA	CBA-CGA-O2A-C1
24	BG	401	CLA	CBA-CGA-O2A-C1
24	BJ	603	CLA	CBA-CGA-O2A-C1
24	BJ	611	CLA	CBA-CGA-O2A-C1
24	BQ	603	CLA	CBA-CGA-O2A-C1
24	BQ	613	CLA	CBA-CGA-O2A-C1
24	Ba	303	CLA	CBA-CGA-O2A-C1
24	Ba	311	CLA	CBA-CGA-O2A-C1
24	BF	511	CLA	CBA-CGA-O2A-C1
24	BU	608	CLA	CBA-CGA-O2A-C1
27	BF	520	LHG	C24-C23-O8-C6
32	L	103	SQD	C24-C23-O48-C46
32	a	412	SQD	C24-C23-O48-C46
32	A1	101	SQD	C24-C23-O48-C46
32	BD	412	SQD	C24-C23-O48-C46
34	1	517	DGD	C2A-C1A-O1G-C1G
38	a	409	PHO	CBA-CGA-O2A-C1
38	BD	409	PHO	CBA-CGA-O2A-C1
24	BE	607	CLA	C8-C10-C11-C12
34	BD	413	DGD	O6E-C5E-C6E-O5E
24	A	407	CLA	CBD-CGD-O2D-CED
24	0	614	CLA	CBD-CGD-O2D-CED
30	Aw	101	LMG	C4-C5-C6-O5
23	G	609	CHL	C2C-C3C-CAC-CBC
24	7	305	CLA	O1D-CGD-O2D-CED
24	AA	305	CLA	O1D-CGD-O2D-CED
24	v	607	CLA	O1D-CGD-O2D-CED
26	5	617	NEX	C13-C14-C15-C35
26	N	617	NEX	C13-C14-C15-C35
26	9	617	NEX	C13-C14-C15-C35
26	A2	617	NEX	C13-C14-C15-C35
26	BB	320	NEX	C9-C10-C11-C12
26	BV	616	NEX	C9-C10-C11-C12
29	8	313	BCR	C19-C20-C21-C22
29	AB	313	BCR	C19-C20-C21-C22
27	D	404	LHG	C24-C25-C26-C27
32	BD	412	SQD	C17-C18-C19-C20
23	G	608	CHL	C13-C15-C16-C17
23	Au	608	CHL	C13-C15-C16-C17
24	g	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C13-C15-C16-C17
24	C	513	CLA	C8-C10-C11-C12
24	0	610	CLA	C10-C11-C12-C13
24	v	613	CLA	C10-C11-C12-C13
24	BB	313	CLA	C5-C6-C7-C8
24	1	512	CLA	C10-C11-C12-C13
24	1	513	CLA	C8-C10-C11-C12
23	Ba	310	CHL	C2C-C3C-CAC-CBC
32	a	412	SQD	C17-C18-C19-C20
24	n	603	CLA	O1D-CGD-O2D-CED
24	BD	406	CLA	O1D-CGD-O2D-CED
23	BJ	607	CHL	C2C-C3C-CAC-CBC
30	I	101	LMG	C4-C5-C6-O5
23	Y	302	CHL	C15-C16-C17-C18
23	g	607	CHL	C13-C15-C16-C17
23	n	601	CHL	C15-C16-C17-C18
23	BB	302	CHL	C15-C16-C17-C18
23	BJ	607	CHL	C13-C15-C16-C17
23	BQ	601	CHL	C15-C16-C17-C18
24	B	606	CLA	C10-C11-C12-C13
24	B	608	CLA	C5-C6-C7-C8
24	B	613	CLA	C10-C11-C12-C13
24	G	602	CLA	C15-C16-C17-C18
24	I	102	CLA	C15-C16-C17-C18
24	Y	313	CLA	C5-C6-C7-C8
24	b	607	CLA	C8-C10-C11-C12
24	b	609	CLA	C5-C6-C7-C8
24	b	617	CLA	C5-C6-C7-C8
24	b	617	CLA	C15-C16-C17-C18
24	C	512	CLA	C10-C11-C12-C13
24	c	508	CLA	C10-C11-C12-C13
24	c	508	CLA	C13-C15-C16-C17
24	c	514	CLA	C8-C10-C11-C12
24	r	603	CLA	C10-C11-C12-C13
24	v	606	CLA	C8-C10-C11-C12
24	v	606	CLA	C10-C11-C12-C13
24	v	608	CLA	C5-C6-C7-C8
24	BE	614	CLA	C10-C11-C12-C13
24	BE	617	CLA	C5-C6-C7-C8
24	BJ	602	CLA	C5-C6-C7-C8
24	1	507	CLA	C13-C15-C16-C17
24	BF	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	BF	508	CLA	C13-C15-C16-C17
24	BF	514	CLA	C8-C10-C11-C12
27	b	624	LHG	O2-C2-C3-O3
30	B	620	LMG	C28-C29-C30-C31
32	A1	101	SQD	C23-C24-C25-C26
23	N	608	CHL	C3-C5-C6-C7
23	n	608	CHL	C3-C5-C6-C7
23	r	606	CHL	C3-C5-C6-C7
23	A2	608	CHL	C3-C5-C6-C7
23	BQ	608	CHL	C3-C5-C6-C7
23	BU	606	CHL	C3-C5-C6-C7
24	r	604	CLA	O2A-C1-C2-C3
27	c	520	LHG	O7-C5-C6-O8
27	BF	521	LHG	O7-C5-C6-O8
32	a	412	SQD	O6-C44-C45-O47
32	BD	412	SQD	O6-C44-C45-O47
27	Au	618	LHG	C28-C29-C30-C31
23	Au	609	CHL	O1A-CGA-O2A-C1
24	6	602	CLA	O1A-CGA-O2A-C1
24	N	614	CLA	O1A-CGA-O2A-C1
24	b	607	CLA	O1A-CGA-O2A-C1
24	n	603	CLA	O1A-CGA-O2A-C1
24	r	608	CLA	O1A-CGA-O2A-C1
24	r	609	CLA	O1A-CGA-O2A-C1
24	9	613	CLA	O1A-CGA-O2A-C1
24	v	606	CLA	O1A-CGA-O2A-C1
24	BE	607	CLA	O1A-CGA-O2A-C1
24	BJ	603	CLA	O1A-CGA-O2A-C1
24	BQ	603	CLA	O1A-CGA-O2A-C1
24	BU	609	CLA	O1A-CGA-O2A-C1
27	C	520	LHG	O10-C23-O8-C6
27	1	520	LHG	O10-C23-O8-C6
24	v	614	CLA	C4-C3-C5-C6
23	Ba	302	CHL	C2-C3-C5-C6
24	B	607	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	v	607	CLA	C2-C3-C5-C6
23	N	607	CHL	C11-C12-C13-C14
23	N	608	CHL	C14-C13-C15-C16
23	Y	308	CHL	C11-C12-C13-C14
23	Y	309	CHL	C14-C13-C15-C16
23	g	608	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	n	608	CHL	C14-C13-C15-C16
23	y	310	CHL	C14-C13-C15-C16
23	0	601	CHL	C14-C13-C15-C16
23	A2	607	CHL	C11-C12-C13-C14
23	A2	608	CHL	C14-C13-C15-C16
23	BB	308	CHL	C11-C12-C13-C14
23	BB	309	CHL	C14-C13-C15-C16
23	BJ	608	CHL	C14-C13-C15-C16
23	BQ	608	CHL	C14-C13-C15-C16
23	Ba	310	CHL	C14-C13-C15-C16
24	5	602	CLA	C11-C10-C8-C9
24	6	602	CLA	C11-C10-C8-C9
24	B	602	CLA	C6-C7-C8-C9
24	B	604	CLA	C6-C7-C8-C9
24	B	607	CLA	C6-C7-C8-C9
24	B	608	CLA	C6-C7-C8-C9
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C9
24	D	401	CLA	C6-C7-C8-C9
24	G	603	CLA	C6-C7-C8-C9
24	S	602	CLA	C11-C10-C8-C9
24	Y	303	CLA	C11-C10-C8-C9
24	Y	303	CLA	C14-C13-C15-C16
24	b	603	CLA	C6-C7-C8-C9
24	b	604	CLA	C14-C13-C15-C16
24	b	605	CLA	C6-C7-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	b	608	CLA	C6-C7-C8-C9
24	b	615	CLA	C14-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C9
24	d	401	CLA	C6-C7-C8-C9
24	n	602	CLA	C11-C10-C8-C9
24	n	603	CLA	C6-C7-C8-C9
24	n	611	CLA	C11-C10-C8-C9
24	s	602	CLA	C11-C10-C8-C9
24	y	303	CLA	C14-C13-C15-C16
24	y	312	CLA	C11-C10-C8-C9
24	C	502	CLA	C14-C13-C15-C16
24	C	504	CLA	C11-C10-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	C6-C7-C8-C9
24	C	513	CLA	C14-C13-C15-C16
24	c	502	CLA	C14-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	c	514	CLA	C14-C13-C15-C16
24	9	602	CLA	C11-C10-C8-C9
24	0	602	CLA	C11-C10-C8-C9
24	v	602	CLA	C6-C7-C8-C9
24	v	604	CLA	C6-C7-C8-C9
24	v	607	CLA	C6-C7-C8-C9
24	v	608	CLA	C6-C7-C8-C9
24	v	614	CLA	C14-C13-C15-C16
24	2	402	CLA	C6-C7-C8-C9
24	Au	603	CLA	C6-C7-C8-C9
24	A6	602	CLA	C11-C10-C8-C9
24	BB	303	CLA	C11-C10-C8-C9
24	BB	303	CLA	C14-C13-C15-C16
24	BE	603	CLA	C6-C7-C8-C9
24	BE	604	CLA	C14-C13-C15-C16
24	BE	605	CLA	C6-C7-C8-C9
24	BE	606	CLA	C14-C13-C15-C16
24	BE	607	CLA	C11-C12-C13-C14
24	BE	608	CLA	C6-C7-C8-C9
24	BE	615	CLA	C14-C13-C15-C16
24	BE	616	CLA	C11-C10-C8-C9
24	BG	401	CLA	C6-C7-C8-C9
24	BQ	602	CLA	C11-C10-C8-C9
24	BQ	603	CLA	C6-C7-C8-C9
24	BQ	611	CLA	C11-C10-C8-C9
24	BV	602	CLA	C11-C10-C8-C9
24	Ba	303	CLA	C14-C13-C15-C16
24	Ba	312	CLA	C11-C10-C8-C9
24	1	502	CLA	C14-C13-C15-C16
24	1	504	CLA	C11-C10-C8-C9
24	1	506	CLA	C11-C12-C13-C14
24	1	507	CLA	C11-C10-C8-C9
24	1	509	CLA	C6-C7-C8-C9
24	1	513	CLA	C14-C13-C15-C16
24	BF	502	CLA	C14-C13-C15-C16
24	BF	504	CLA	C11-C10-C8-C9
24	BF	508	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	BF	510	CLA	C6-C7-C8-C9
24	BF	514	CLA	C14-C13-C15-C16
38	A	409	PHO	C6-C7-C8-C9
38	R	407	PHO	C14-C13-C15-C16
38	R	408	PHO	C6-C7-C8-C9
38	BD	409	PHO	C6-C7-C8-C9
23	BV	605	CHL	O1D-CGD-O2D-CED
24	b	611	CLA	O1D-CGD-O2D-CED
24	g	612	CLA	O1D-CGD-O2D-CED
24	BE	612	CLA	O1D-CGD-O2D-CED
24	BJ	612	CLA	O1D-CGD-O2D-CED
38	A	409	PHO	O1D-CGD-O2D-CED
24	b	615	CLA	CBD-CGD-O2D-CED
24	s	612	CLA	CBD-CGD-O2D-CED
23	0	607	CHL	C2C-C3C-CAC-CBC
23	BJ	609	CHL	C4C-C3C-CAC-CBC
27	G	618	LHG	C28-C29-C30-C31
24	S	609	CLA	C5-C6-C7-C8
24	b	614	CLA	C10-C11-C12-C13
24	v	611	CLA	C8-C10-C11-C12
24	Aw	102	CLA	C15-C16-C17-C18
24	BE	609	CLA	C5-C6-C7-C8
23	BJ	609	CHL	C2A-CAA-CBA-CGA
23	BQ	607	CHL	C2A-CAA-CBA-CGA
24	6	602	CLA	C2A-CAA-CBA-CGA
24	s	602	CLA	C2A-CAA-CBA-CGA
24	A	410	CLA	C2A-CAA-CBA-CGA
24	c	502	CLA	C2A-CAA-CBA-CGA
24	0	602	CLA	C2A-CAA-CBA-CGA
24	1	511	CLA	C2A-CAA-CBA-CGA
24	BF	502	CLA	C2A-CAA-CBA-CGA
25	5	615	LUT	C7-C8-C9-C19
25	S	614	LUT	C7-C8-C9-C19
25	y	316	LUT	C7-C8-C9-C19
25	r	615	LUT	C7-C8-C9-C19
25	9	615	LUT	C7-C8-C9-C19
25	0	615	LUT	C7-C8-C9-C19
25	A6	614	LUT	C7-C8-C9-C19
25	BU	615	LUT	C7-C8-C9-C19
26	G	617	NEX	C27-C28-C29-C39
26	r	617	NEX	C11-C12-C13-C20
26	9	617	NEX	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
26	BJ	617	NEX	C11-C12-C13-C20
28	7	301	XAT	C7-C8-C9-C19
28	G	619	XAT	C7-C8-C9-C19
28	G	619	XAT	C11-C12-C13-C20
28	N	619	XAT	C11-C12-C13-C20
28	N	619	XAT	C27-C28-C29-C39
28	Y	301	XAT	C7-C8-C9-C19
28	Y	301	XAT	C11-C12-C13-C20
28	g	619	XAT	C7-C8-C9-C19
28	g	619	XAT	C11-C12-C13-C20
28	r	616	XAT	C11-C12-C13-C20
28	9	619	XAT	C31-C32-C33-C40
28	AA	301	XAT	C7-C8-C9-C19
28	Au	619	XAT	C7-C8-C9-C19
28	Au	619	XAT	C11-C12-C13-C20
28	A2	619	XAT	C11-C12-C13-C20
28	A2	619	XAT	C27-C28-C29-C39
28	BB	301	XAT	C7-C8-C9-C19
28	BB	301	XAT	C11-C12-C13-C20
28	BJ	619	XAT	C7-C8-C9-C19
28	BJ	619	XAT	C11-C12-C13-C20
28	BQ	619	XAT	C31-C32-C33-C40
28	Ba	301	XAT	C11-C12-C13-C20
28	BU	616	XAT	C11-C12-C13-C20
29	K	101	BCR	C7-C8-C9-C34
29	K	101	BCR	C37-C22-C23-C24
29	k	101	BCR	C37-C22-C23-C24
29	A	411	BCR	C7-C8-C9-C34
29	a	411	BCR	C7-C8-C9-C34
29	Ay	101	BCR	C7-C8-C9-C34
29	Ay	101	BCR	C37-C22-C23-C24
29	BN	101	BCR	C7-C8-C9-C34
29	BN	101	BCR	C37-C22-C23-C24
29	Bb	101	BCR	C7-C8-C9-C34
25	5	615	LUT	C7-C8-C9-C10
25	9	615	LUT	C7-C8-C9-C10
26	r	617	NEX	C11-C12-C13-C14
26	BB	320	NEX	C11-C12-C13-C14
28	AA	301	XAT	C31-C32-C33-C34
29	8	313	BCR	C21-C22-C23-C24
29	B	623	BCR	C7-C8-C9-C10
29	K	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	k	101	BCR	C7-C8-C9-C10
29	AB	313	BCR	C21-C22-C23-C24
29	Ay	101	BCR	C7-C8-C9-C10
34	A	402	DGD	C2B-C1B-O2G-C2G
30	c	501	LMG	C10-C11-C12-C13
30	v	620	LMG	C28-C29-C30-C31
30	BF	501	LMG	C10-C11-C12-C13
32	D	406	SQD	C23-C24-C25-C26
32	L	103	SQD	C23-C24-C25-C26
34	h	102	DGD	O6D-C5D-C6D-O5D
34	BK	102	DGD	O6D-C5D-C6D-O5D
23	6	601	CHL	O1A-CGA-O2A-C1
23	r	607	CHL	O1A-CGA-O2A-C1
23	BB	310	CHL	O1A-CGA-O2A-C1
23	BU	607	CHL	O1A-CGA-O2A-C1
24	B	606	CLA	O1A-CGA-O2A-C1
24	B	612	CLA	O1A-CGA-O2A-C1
24	I	102	CLA	O1A-CGA-O2A-C1
24	S	604	CLA	O1A-CGA-O2A-C1
24	b	602	CLA	O1A-CGA-O2A-C1
24	g	603	CLA	O1A-CGA-O2A-C1
24	0	602	CLA	O1A-CGA-O2A-C1
24	Aw	102	CLA	O1A-CGA-O2A-C1
24	A2	614	CLA	O1A-CGA-O2A-C1
24	BE	602	CLA	O1A-CGA-O2A-C1
24	BG	401	CLA	O1A-CGA-O2A-C1
24	Ba	311	CLA	O1A-CGA-O2A-C1
24	BU	608	CLA	O1A-CGA-O2A-C1
23	Y	308	CHL	C15-C16-C17-C18
23	n	609	CHL	C15-C16-C17-C18
23	Au	607	CHL	C13-C15-C16-C17
23	BJ	601	CHL	C13-C15-C16-C17
23	BQ	601	CHL	C13-C15-C16-C17
23	BQ	607	CHL	C15-C16-C17-C18
24	B	616	CLA	C15-C16-C17-C18
24	b	603	CLA	C5-C6-C7-C8
24	b	607	CLA	C10-C11-C12-C13
24	b	615	CLA	C8-C10-C11-C12
24	n	611	CLA	C8-C10-C11-C12
24	v	602	CLA	C5-C6-C7-C8
24	v	607	CLA	C13-C15-C16-C17
24	v	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	Au	602	CLA	C15-C16-C17-C18
24	A6	609	CLA	C5-C6-C7-C8
24	BE	615	CLA	C8-C10-C11-C12
24	BQ	611	CLA	C8-C10-C11-C12
24	1	513	CLA	C15-C16-C17-C18
38	a	408	PHO	C13-C15-C16-C17
24	B	607	CLA	O1D-CGD-O2D-CED
24	BQ	603	CLA	O1D-CGD-O2D-CED
24	Ba	303	CLA	O1D-CGD-O2D-CED
24	R	409	CLA	O1D-CGD-O2D-CED
23	g	609	CHL	C4C-C3C-CAC-CBC
24	b	612	CLA	O1D-CGD-O2D-CED
23	G	601	CHL	C10-C11-C12-C13
23	Y	302	CHL	C10-C11-C12-C13
23	BB	302	CHL	C10-C11-C12-C13
24	B	607	CLA	CBA-CGA-O2A-C1
24	g	610	CLA	CBA-CGA-O2A-C1
24	s	612	CLA	CBA-CGA-O2A-C1
24	r	601	CLA	CBA-CGA-O2A-C1
24	v	607	CLA	CBA-CGA-O2A-C1
24	BJ	610	CLA	CBA-CGA-O2A-C1
24	BV	612	CLA	CBA-CGA-O2A-C1
24	BU	601	CLA	CBA-CGA-O2A-C1
27	c	519	LHG	C24-C23-O8-C6
23	BJ	608	CHL	C13-C15-C16-C17
23	BQ	609	CHL	C15-C16-C17-C18
24	6	610	CLA	C10-C11-C12-C13
24	B	606	CLA	C5-C6-C7-C8
24	B	614	CLA	C8-C10-C11-C12
24	G	603	CLA	C13-C15-C16-C17
24	N	610	CLA	C15-C16-C17-C18
24	b	614	CLA	C8-C10-C11-C12
24	c	506	CLA	C15-C16-C17-C18
24	v	606	CLA	C5-C6-C7-C8
24	v	616	CLA	C15-C16-C17-C18
24	2	402	CLA	C15-C16-C17-C18
24	A2	610	CLA	C15-C16-C17-C18
24	BE	607	CLA	C10-C11-C12-C13
24	BE	612	CLA	C8-C10-C11-C12
24	BE	615	CLA	C10-C11-C12-C13
24	BE	617	CLA	C15-C16-C17-C18
24	BQ	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	BF	506	CLA	C15-C16-C17-C18
24	BF	514	CLA	C15-C16-C17-C18
24	BU	603	CLA	C10-C11-C12-C13
38	BD	408	PHO	C13-C15-C16-C17
30	2	407	LMG	O6-C5-C6-O5
34	A	402	DGD	O6E-C5E-C6E-O5E
34	R	401	DGD	O6E-C5E-C6E-O5E
27	6	617	LHG	C23-C24-C25-C26
27	b	623	LHG	C23-C24-C25-C26
27	b	624	LHG	C23-C24-C25-C26
27	c	519	LHG	C23-C24-C25-C26
27	BE	623	LHG	C23-C24-C25-C26
27	BF	521	LHG	C23-C24-C25-C26
30	b	621	LMG	C28-C29-C30-C31
32	2	408	SQD	C23-C24-C25-C26
24	y	303	CLA	O1D-CGD-O2D-CED
24	v	612	CLA	O1A-CGA-O2A-C1
23	A6	605	CHL	O1D-CGD-O2D-CED
23	N	607	CHL	C15-C16-C17-C18
23	g	608	CHL	C13-C15-C16-C17
23	n	607	CHL	C15-C16-C17-C18
23	y	308	CHL	C15-C16-C17-C18
23	A2	607	CHL	C15-C16-C17-C18
23	BB	308	CHL	C15-C16-C17-C18
23	BQ	608	CHL	C15-C16-C17-C18
23	Ba	308	CHL	C15-C16-C17-C18
24	6	613	CLA	C8-C10-C11-C12
24	B	606	CLA	C8-C10-C11-C12
24	B	611	CLA	C8-C10-C11-C12
24	D	401	CLA	C15-C16-C17-C18
24	G	602	CLA	C5-C6-C7-C8
24	G	603	CLA	C15-C16-C17-C18
24	b	604	CLA	C13-C15-C16-C17
24	b	612	CLA	C8-C10-C11-C12
24	g	603	CLA	C15-C16-C17-C18
24	n	610	CLA	C5-C6-C7-C8
24	n	610	CLA	C15-C16-C17-C18
24	C	513	CLA	C15-C16-C17-C18
24	c	511	CLA	C13-C15-C16-C17
24	c	513	CLA	C10-C11-C12-C13
24	c	514	CLA	C15-C16-C17-C18
24	0	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	Au	602	CLA	C5-C6-C7-C8
24	Au	603	CLA	C15-C16-C17-C18
24	BE	603	CLA	C5-C6-C7-C8
24	BE	613	CLA	C15-C16-C17-C18
24	BE	614	CLA	C8-C10-C11-C12
24	BJ	603	CLA	C15-C16-C17-C18
24	BQ	610	CLA	C15-C16-C17-C18
24	BF	507	CLA	C13-C15-C16-C17
24	BF	511	CLA	C13-C15-C16-C17
24	BF	513	CLA	C10-C11-C12-C13
23	AB	307	CHL	C2C-C3C-CAC-CBC
27	d	404	LHG	C28-C29-C30-C31
23	s	607	CHL	O1D-CGD-O2D-CED
24	N	602	CLA	O1D-CGD-O2D-CED
27	c	520	LHG	O1-C1-C2-O2
27	BF	521	LHG	O1-C1-C2-O2
24	B	601	CLA	O1A-CGA-O2A-C1
24	G	603	CLA	O1A-CGA-O2A-C1
27	B	622	LHG	C23-C24-C25-C26
27	G	618	LHG	C23-C24-C25-C26
27	L	102	LHG	C23-C24-C25-C26
27	C	520	LHG	C23-C24-C25-C26
27	c	520	LHG	C23-C24-C25-C26
27	0	617	LHG	C23-C24-C25-C26
27	2	405	LHG	C23-C24-C25-C26
27	Au	618	LHG	C23-C24-C25-C26
27	Az	102	LHG	C23-C24-C25-C26
27	A2	618	LHG	C23-C24-C25-C26
27	BE	624	LHG	C23-C24-C25-C26
27	1	520	LHG	C23-C24-C25-C26
27	BF	520	LHG	C23-C24-C25-C26
32	d	406	SQD	C23-C24-C25-C26
32	l	101	SQD	C23-C24-C25-C26
32	BG	406	SQD	C23-C24-C25-C26
30	D	405	LMG	O6-C5-C6-O5
27	BG	404	LHG	C28-C29-C30-C31
34	a	413	DGD	C4E-C5E-C6E-O5E
24	A	410	CLA	O1D-CGD-O2D-CED
23	g	601	CHL	C13-C15-C16-C17
23	n	608	CHL	C15-C16-C17-C18
23	y	309	CHL	C15-C16-C17-C18
23	r	605	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	BJ	601	CHL	C15-C16-C17-C18
23	Ba	309	CHL	C15-C16-C17-C18
23	BU	605	CHL	C13-C15-C16-C17
24	B	614	CLA	C13-C15-C16-C17
24	b	611	CLA	C15-C16-C17-C18
24	b	615	CLA	C10-C11-C12-C13
24	g	610	CLA	C5-C6-C7-C8
24	n	611	CLA	C5-C6-C7-C8
24	C	507	CLA	C10-C11-C12-C13
24	c	504	CLA	C5-C6-C7-C8
24	c	504	CLA	C15-C16-C17-C18
24	c	507	CLA	C13-C15-C16-C17
24	v	614	CLA	C13-C15-C16-C17
24	Au	603	CLA	C13-C15-C16-C17
24	BE	611	CLA	C15-C16-C17-C18
24	BJ	610	CLA	C5-C6-C7-C8
24	R	409	CLA	C8-C10-C11-C12
24	1	504	CLA	C5-C6-C7-C8
38	R	407	PHO	C13-C15-C16-C17
24	6	614	CLA	CBA-CGA-O2A-C1
24	G	613	CLA	CBA-CGA-O2A-C1
24	0	614	CLA	CBA-CGA-O2A-C1
24	Au	613	CLA	CBA-CGA-O2A-C1
38	A	409	PHO	CBA-CGA-O2A-C1
24	B	610	CLA	O1D-CGD-O2D-CED
24	B	611	CLA	O1D-CGD-O2D-CED
24	b	610	CLA	O1D-CGD-O2D-CED
24	BE	611	CLA	O1D-CGD-O2D-CED
23	g	601	CHL	C15-C16-C17-C18
23	r	605	CHL	C15-C16-C17-C18
23	BU	605	CHL	C15-C16-C17-C18
24	B	607	CLA	C13-C15-C16-C17
24	A	410	CLA	C8-C10-C11-C12
24	C	504	CLA	C5-C6-C7-C8
24	BQ	611	CLA	C5-C6-C7-C8
24	1	507	CLA	C10-C11-C12-C13
24	BF	504	CLA	C5-C6-C7-C8
24	BF	504	CLA	C15-C16-C17-C18
38	a	409	PHO	O1A-CGA-O2A-C1
38	BD	409	PHO	O1A-CGA-O2A-C1
23	BB	310	CHL	O1D-CGD-O2D-CED
27	N	618	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	W	201	LHG	C23-C24-C25-C26
27	n	618	LHG	C23-C24-C25-C26
27	w	201	LHG	C23-C24-C25-C26
27	C	521	LHG	C23-C24-C25-C26
27	A0	202	LHG	C23-C24-C25-C26
27	BQ	618	LHG	C23-C24-C25-C26
27	BY	201	LHG	C23-C24-C25-C26
27	1	521	LHG	C23-C24-C25-C26
30	BE	621	LMG	C28-C29-C30-C31
32	A	413	SQD	C7-C8-C9-C10
32	BO	101	SQD	C23-C24-C25-C26
32	R	411	SQD	C7-C8-C9-C10
23	BJ	601	CHL	CBD-CGD-O2D-CED
24	BB	303	CLA	CBD-CGD-O2D-CED
24	BE	615	CLA	CBD-CGD-O2D-CED
23	5	607	CHL	C13-C15-C16-C17
23	6	601	CHL	C10-C11-C12-C13
23	7	308	CHL	C10-C11-C12-C13
23	n	601	CHL	C10-C11-C12-C13
23	9	607	CHL	C13-C15-C16-C17
23	AA	308	CHL	C10-C11-C12-C13
23	Au	601	CHL	C10-C11-C12-C13
23	BQ	601	CHL	C10-C11-C12-C13
23	Ba	302	CHL	C10-C11-C12-C13
23	BU	607	CHL	C10-C11-C12-C13
34	R	401	DGD	C2B-C1B-O2G-C2G
23	G	608	CHL	C3-C5-C6-C7
23	Au	608	CHL	C3-C5-C6-C7
24	BU	604	CLA	O2A-C1-C2-C3
23	Y	309	CHL	C15-C16-C17-C18
23	n	601	CHL	C13-C15-C16-C17
24	b	613	CLA	C15-C16-C17-C18
24	C	504	CLA	C15-C16-C17-C18
24	C	506	CLA	C15-C16-C17-C18
24	Ba	313	CLA	C5-C6-C7-C8
24	1	506	CLA	C15-C16-C17-C18
23	N	608	CHL	C12-C13-C15-C16
23	A2	608	CHL	C12-C13-C15-C16
23	BB	309	CHL	C12-C13-C15-C16
24	Y	303	CLA	C6-C7-C8-C10
24	b	603	CLA	C6-C7-C8-C10
24	BF	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	BF	506	CLA	C11-C10-C8-C7
23	G	601	CHL	O1A-CGA-O2A-C1
23	Y	302	CHL	O1A-CGA-O2A-C1
23	Au	601	CHL	O1A-CGA-O2A-C1
23	BB	302	CHL	O1A-CGA-O2A-C1
23	Ba	302	CHL	O1A-CGA-O2A-C1
24	D	401	CLA	O1A-CGA-O2A-C1
24	g	611	CLA	O1A-CGA-O2A-C1
24	n	613	CLA	O1A-CGA-O2A-C1
24	v	601	CLA	O1A-CGA-O2A-C1
24	2	402	CLA	O1A-CGA-O2A-C1
24	Au	603	CLA	O1A-CGA-O2A-C1
24	BE	613	CLA	O1A-CGA-O2A-C1
24	BJ	611	CLA	O1A-CGA-O2A-C1
24	BQ	613	CLA	O1A-CGA-O2A-C1
32	a	412	SQD	O10-C23-O48-C46
32	BD	412	SQD	O10-C23-O48-C46
23	y	310	CHL	C2C-C3C-CAC-CBC
26	S	616	NEX	C9-C10-C11-C12
26	s	616	NEX	C9-C10-C11-C12
26	r	617	NEX	C9-C10-C11-C12
26	A6	616	NEX	C9-C10-C11-C12
26	A6	616	NEX	C13-C14-C15-C35
26	BB	318	NEX	C29-C30-C31-C32
26	BQ	617	NEX	C13-C14-C15-C35
28	r	616	XAT	C9-C10-C11-C12
28	BU	616	XAT	C9-C10-C11-C12
23	n	609	CHL	C2A-CAA-CBA-CGA
23	9	607	CHL	C2A-CAA-CBA-CGA
23	BQ	609	CHL	C2A-CAA-CBA-CGA
24	6	610	CLA	C2A-CAA-CBA-CGA
24	B	607	CLA	C2A-CAA-CBA-CGA
24	N	611	CLA	C2A-CAA-CBA-CGA
24	S	610	CLA	C2A-CAA-CBA-CGA
24	Y	303	CLA	C2A-CAA-CBA-CGA
24	Y	305	CLA	C2A-CAA-CBA-CGA
24	b	602	CLA	C2A-CAA-CBA-CGA
24	b	608	CLA	C2A-CAA-CBA-CGA
24	g	613	CLA	C2A-CAA-CBA-CGA
24	a	410	CLA	C2A-CAA-CBA-CGA
24	0	603	CLA	C2A-CAA-CBA-CGA
24	v	607	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	BB	305	CLA	C2A-CAA-CBA-CGA
24	BE	602	CLA	C2A-CAA-CBA-CGA
24	BE	608	CLA	C2A-CAA-CBA-CGA
24	Ba	303	CLA	C2A-CAA-CBA-CGA
24	Ba	311	CLA	C2A-CAA-CBA-CGA
24	BD	410	CLA	C2A-CAA-CBA-CGA
24	BF	509	CLA	C2A-CAA-CBA-CGA
24	BU	614	CLA	C2A-CAA-CBA-CGA
23	S	605	CHL	O1D-CGD-O2D-CED
24	G	612	CLA	O1D-CGD-O2D-CED
24	b	608	CLA	O1D-CGD-O2D-CED
24	9	603	CLA	O1D-CGD-O2D-CED
24	v	611	CLA	O1D-CGD-O2D-CED
24	A2	602	CLA	O1D-CGD-O2D-CED
24	BE	608	CLA	O1D-CGD-O2D-CED
24	BF	508	CLA	O1D-CGD-O2D-CED
23	N	608	CHL	C15-C16-C17-C18
23	N	609	CHL	C15-C16-C17-C18
23	y	302	CHL	C15-C16-C17-C18
23	BB	309	CHL	C15-C16-C17-C18
23	Ba	302	CHL	C15-C16-C17-C18
24	B	607	CLA	C5-C6-C7-C8
24	B	612	CLA	C10-C11-C12-C13
24	b	607	CLA	C5-C6-C7-C8
24	b	608	CLA	C8-C10-C11-C12
24	b	608	CLA	C13-C15-C16-C17
24	b	613	CLA	C10-C11-C12-C13
24	g	603	CLA	C13-C15-C16-C17
24	y	313	CLA	C5-C6-C7-C8
24	C	510	CLA	C13-C15-C16-C17
24	a	410	CLA	C8-C10-C11-C12
24	v	607	CLA	C5-C6-C7-C8
24	Aw	102	CLA	C5-C6-C7-C8
24	BE	608	CLA	C13-C15-C16-C17
24	BE	613	CLA	C10-C11-C12-C13
24	BJ	603	CLA	C13-C15-C16-C17
24	1	504	CLA	C15-C16-C17-C18
24	BD	410	CLA	C8-C10-C11-C12
24	BU	603	CLA	C5-C6-C7-C8
38	A	408	PHO	C13-C15-C16-C17
23	5	601	CHL	C4C-C3C-CAC-CBC
29	b	601	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	y	302	CHL	O1A-CGA-O2A-C1
24	5	602	CLA	O1A-CGA-O2A-C1
24	B	615	CLA	O1A-CGA-O2A-C1
24	G	610	CLA	O1A-CGA-O2A-C1
24	N	603	CLA	O1A-CGA-O2A-C1
24	b	608	CLA	O1A-CGA-O2A-C1
24	b	613	CLA	O1A-CGA-O2A-C1
24	Au	610	CLA	O1A-CGA-O2A-C1
24	A2	603	CLA	O1A-CGA-O2A-C1
24	A6	604	CLA	O1A-CGA-O2A-C1
24	A6	612	CLA	O1A-CGA-O2A-C1
24	BE	603	CLA	O1A-CGA-O2A-C1
24	BE	608	CLA	O1A-CGA-O2A-C1
24	Ba	303	CLA	O1A-CGA-O2A-C1
32	L	103	SQD	O10-C23-O48-C46
32	A1	101	SQD	O10-C23-O48-C46
23	G	601	CHL	CBD-CGD-O2D-CED
24	A	406	CLA	CBD-CGD-O2D-CED
34	BD	413	DGD	C4E-C5E-C6E-O5E
32	a	412	SQD	O5-C1-O6-C44
32	BD	412	SQD	O5-C1-O6-C44
34	h	102	DGD	O6E-C1E-O5D-C6D
34	BK	102	DGD	O6E-C1E-O5D-C6D
23	y	310	CHL	C13-C15-C16-C17
23	A2	608	CHL	C15-C16-C17-C18
23	A2	609	CHL	C15-C16-C17-C18
23	Ba	310	CHL	C13-C15-C16-C17
24	B	613	CLA	C8-C10-C11-C12
24	N	611	CLA	C8-C10-C11-C12
24	g	602	CLA	C15-C16-C17-C18
24	r	603	CLA	C5-C6-C7-C8
24	v	612	CLA	C10-C11-C12-C13
24	BE	608	CLA	C8-C10-C11-C12
24	Ba	313	CLA	C10-C11-C12-C13
23	G	608	CHL	O1D-CGD-O2D-CED
24	BE	610	CLA	O1D-CGD-O2D-CED
27	g	618	LHG	C23-C24-C25-C26
27	BJ	618	LHG	C23-C24-C25-C26
26	5	617	NEX	C10-C11-C12-C13
26	7	319	NEX	C30-C31-C32-C33
26	y	318	NEX	C10-C11-C12-C13
26	r	617	NEX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	9	617	NEX	C10-C11-C12-C13
26	BB	320	NEX	C10-C11-C12-C13
26	Ba	318	NEX	C10-C11-C12-C13
28	8	312	XAT	C10-C11-C12-C13
28	y	301	XAT	C10-C11-C12-C13
28	AB	312	XAT	C10-C11-C12-C13
28	Ba	301	XAT	C10-C11-C12-C13
29	v	622	BCR	C18-C19-C20-C21
27	B	622	LHG	O2-C2-C3-O3
27	b	623	LHG	O2-C2-C3-O3
27	2	405	LHG	O2-C2-C3-O3
27	BE	623	LHG	O2-C2-C3-O3
27	BE	624	LHG	O2-C2-C3-O3
24	B	613	CLA	C3-C5-C6-C7
24	g	610	CLA	C3-C5-C6-C7
24	C	507	CLA	C3-C5-C6-C7
24	v	614	CLA	C3-C5-C6-C7
24	BJ	610	CLA	C3-C5-C6-C7
24	1	510	CLA	C3-C5-C6-C7
23	y	302	CHL	C10-C11-C12-C13
23	r	607	CHL	C10-C11-C12-C13
23	0	601	CHL	C10-C11-C12-C13
23	G	607	CHL	C13-C15-C16-C17
24	B	601	CLA	C10-C11-C12-C13
24	B	610	CLA	C13-C15-C16-C17
24	B	612	CLA	C15-C16-C17-C18
24	I	102	CLA	C5-C6-C7-C8
24	b	602	CLA	C10-C11-C12-C13
24	b	608	CLA	C10-C11-C12-C13
24	b	611	CLA	C13-C15-C16-C17
24	y	313	CLA	C10-C11-C12-C13
24	C	510	CLA	C10-C11-C12-C13
24	0	611	CLA	C5-C6-C7-C8
24	v	601	CLA	C10-C11-C12-C13
24	BE	602	CLA	C10-C11-C12-C13
24	BE	607	CLA	C5-C6-C7-C8
24	BE	608	CLA	C10-C11-C12-C13
24	BE	611	CLA	C13-C15-C16-C17
24	BE	616	CLA	C8-C10-C11-C12
24	BJ	602	CLA	C15-C16-C17-C18
24	1	510	CLA	C10-C11-C12-C13
24	r	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	9	601	CHL	C4C-C3C-CAC-CBC
23	6	607	CHL	O1A-CGA-O2A-C1
23	g	601	CHL	O1A-CGA-O2A-C1
23	0	607	CHL	O1A-CGA-O2A-C1
23	BJ	601	CHL	O1A-CGA-O2A-C1
24	S	612	CLA	O1A-CGA-O2A-C1
24	b	603	CLA	O1A-CGA-O2A-C1
24	s	612	CLA	O1A-CGA-O2A-C1
24	y	303	CLA	O1A-CGA-O2A-C1
24	c	511	CLA	O1A-CGA-O2A-C1
24	9	602	CLA	O1A-CGA-O2A-C1
24	v	615	CLA	O1A-CGA-O2A-C1
24	BJ	610	CLA	O1A-CGA-O2A-C1
24	BF	511	CLA	O1A-CGA-O2A-C1
24	BU	601	CLA	O1A-CGA-O2A-C1
32	A	413	SQD	O10-C23-O48-C46
32	R	411	SQD	O10-C23-O48-C46
32	a	412	SQD	C7-C8-C9-C10
32	BD	412	SQD	C7-C8-C9-C10
23	N	608	CHL	C13-C15-C16-C17
23	Y	309	CHL	C13-C15-C16-C17
23	n	608	CHL	C13-C15-C16-C17
23	y	309	CHL	C13-C15-C16-C17
23	A2	608	CHL	C13-C15-C16-C17
23	BB	309	CHL	C13-C15-C16-C17
23	BQ	608	CHL	C13-C15-C16-C17
23	Ba	309	CHL	C13-C15-C16-C17
24	B	603	CLA	C13-C15-C16-C17
24	B	609	CLA	C5-C6-C7-C8
24	N	603	CLA	C15-C16-C17-C18
24	b	604	CLA	C15-C16-C17-C18
24	b	609	CLA	C15-C16-C17-C18
24	s	609	CLA	C5-C6-C7-C8
24	A	410	CLA	C10-C11-C12-C13
24	C	505	CLA	C13-C15-C16-C17
24	0	602	CLA	C10-C11-C12-C13
24	v	616	CLA	C5-C6-C7-C8
24	A2	611	CLA	C8-C10-C11-C12
24	BE	604	CLA	C15-C16-C17-C18
24	BE	610	CLA	C5-C6-C7-C8
24	BV	609	CLA	C5-C6-C7-C8
24	R	409	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	BF	507	CLA	C5-C6-C7-C8
24	BU	609	CLA	C5-C6-C7-C8
23	g	601	CHL	CBD-CGD-O2D-CED
24	6	614	CLA	O1A-CGA-O2A-C1
24	g	610	CLA	O1A-CGA-O2A-C1
24	r	601	CLA	O1A-CGA-O2A-C1
34	c	517	DGD	O1A-C1A-O1G-C1G
34	1	518	DGD	O1A-C1A-O1G-C1G
23	5	607	CHL	O1D-CGD-O2D-CED
23	g	608	CHL	C15-C16-C17-C18
23	BJ	608	CHL	C15-C16-C17-C18
24	6	611	CLA	C5-C6-C7-C8
24	B	602	CLA	C5-C6-C7-C8
24	B	603	CLA	C15-C16-C17-C18
24	B	614	CLA	C10-C11-C12-C13
24	B	616	CLA	C5-C6-C7-C8
24	b	610	CLA	C5-C6-C7-C8
24	d	401	CLA	C15-C16-C17-C18
24	n	603	CLA	C15-C16-C17-C18
24	c	506	CLA	C5-C6-C7-C8
24	c	507	CLA	C5-C6-C7-C8
24	r	609	CLA	C5-C6-C7-C8
24	v	603	CLA	C13-C15-C16-C17
24	v	603	CLA	C15-C16-C17-C18
24	v	609	CLA	C5-C6-C7-C8
24	v	610	CLA	C15-C16-C17-C18
24	v	612	CLA	C15-C16-C17-C18
24	v	614	CLA	C10-C11-C12-C13
24	A2	603	CLA	C15-C16-C17-C18
24	BE	609	CLA	C15-C16-C17-C18
24	1	505	CLA	C13-C15-C16-C17
24	BF	506	CLA	C5-C6-C7-C8
27	W	201	LHG	C3-O3-P-O6
27	b	622	LHG	C4-O6-P-O3
27	n	618	LHG	C3-O3-P-O6
27	w	201	LHG	C3-O3-P-O6
27	C	520	LHG	C3-O3-P-O6
27	C	521	LHG	C3-O3-P-O6
27	c	519	LHG	C3-O3-P-O6
27	c	520	LHG	C3-O3-P-O6
27	r	618	LHG	C3-O3-P-O6
27	A0	202	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
27	BE	622	LHG	C4-O6-P-O3
27	BQ	618	LHG	C3-O3-P-O6
27	BY	201	LHG	C3-O3-P-O6
27	1	520	LHG	C3-O3-P-O6
27	1	521	LHG	C3-O3-P-O6
27	BF	520	LHG	C3-O3-P-O6
27	BF	521	LHG	C3-O3-P-O6
27	BU	617	LHG	C3-O3-P-O6
27	BF	521	LHG	C7-C8-C9-C10
24	C	510	CLA	C3-C5-C6-C7
24	BF	504	CLA	C3-C5-C6-C7
38	A	409	PHO	C3-C5-C6-C7
24	6	611	CLA	CBA-CGA-O2A-C1
24	g	613	CLA	CBA-CGA-O2A-C1
24	y	311	CLA	CBA-CGA-O2A-C1
24	C	504	CLA	CBA-CGA-O2A-C1
24	BU	611	CLA	CBA-CGA-O2A-C1
38	R	408	PHO	CBA-CGA-O2A-C1
23	N	601	CHL	C13-C15-C16-C17
24	b	616	CLA	C8-C10-C11-C12
24	v	610	CLA	C13-C15-C16-C17
24	v	613	CLA	C8-C10-C11-C12
24	BE	604	CLA	C13-C15-C16-C17
24	BG	401	CLA	C15-C16-C17-C18
24	BQ	603	CLA	C15-C16-C17-C18
24	N	603	CLA	O1D-CGD-O2D-CED
24	g	603	CLA	O1D-CGD-O2D-CED
23	N	601	CHL	C10-C11-C12-C13
23	g	601	CHL	C10-C11-C12-C13
23	n	607	CHL	C10-C11-C12-C13
23	A2	601	CHL	C10-C11-C12-C13
23	BJ	601	CHL	C10-C11-C12-C13
27	c	520	LHG	C7-C8-C9-C10
34	h	102	DGD	C1B-C2B-C3B-C4B
23	Au	608	CHL	O1D-CGD-O2D-CED
27	B	622	LHG	C1-C2-C3-O3
27	b	623	LHG	C1-C2-C3-O3
27	C	520	LHG	C1-C2-C3-O3
27	c	519	LHG	C1-C2-C3-O3
27	2	405	LHG	C1-C2-C3-O3
27	BE	623	LHG	C1-C2-C3-O3
27	1	520	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	BF	520	LHG	C1-C2-C3-O3
23	y	308	CHL	C13-C15-C16-C17
24	B	610	CLA	C15-C16-C17-C18
24	AA	303	CLA	C5-C6-C7-C8
24	A6	610	CLA	C5-C6-C7-C8
24	1	510	CLA	C13-C15-C16-C17
24	BJ	603	CLA	O1D-CGD-O2D-CED
24	0	614	CLA	O1A-CGA-O2A-C1
23	G	609	CHL	C4C-C3C-CAC-CBC
23	N	601	CHL	C2A-CAA-CBA-CGA
23	S	607	CHL	C2A-CAA-CBA-CGA
23	s	606	CHL	C2A-CAA-CBA-CGA
23	y	309	CHL	C2A-CAA-CBA-CGA
23	r	606	CHL	C2A-CAA-CBA-CGA
23	A2	601	CHL	C2A-CAA-CBA-CGA
23	BV	606	CHL	C2A-CAA-CBA-CGA
23	Ba	309	CHL	C2A-CAA-CBA-CGA
23	BU	606	CHL	C2A-CAA-CBA-CGA
24	6	603	CLA	C2A-CAA-CBA-CGA
24	G	613	CLA	C2A-CAA-CBA-CGA
24	S	612	CLA	C2A-CAA-CBA-CGA
24	S	613	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
24	d	402	CLA	C2A-CAA-CBA-CGA
24	n	613	CLA	C2A-CAA-CBA-CGA
24	s	610	CLA	C2A-CAA-CBA-CGA
24	s	612	CLA	C2A-CAA-CBA-CGA
24	s	613	CLA	C2A-CAA-CBA-CGA
24	y	303	CLA	C2A-CAA-CBA-CGA
24	y	311	CLA	C2A-CAA-CBA-CGA
24	C	508	CLA	C2A-CAA-CBA-CGA
24	c	509	CLA	C2A-CAA-CBA-CGA
24	r	614	CLA	C2A-CAA-CBA-CGA
24	Au	613	CLA	C2A-CAA-CBA-CGA
24	A6	610	CLA	C2A-CAA-CBA-CGA
24	A6	612	CLA	C2A-CAA-CBA-CGA
24	A6	613	CLA	C2A-CAA-CBA-CGA
24	BB	315	CLA	C2A-CAA-CBA-CGA
24	BE	607	CLA	C2A-CAA-CBA-CGA
24	BJ	613	CLA	C2A-CAA-CBA-CGA
24	BQ	613	CLA	C2A-CAA-CBA-CGA
24	BV	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	BV	612	CLA	C2A-CAA-CBA-CGA
24	BV	613	CLA	C2A-CAA-CBA-CGA
24	R	409	CLA	C2A-CAA-CBA-CGA
24	BF	507	CLA	C2A-CAA-CBA-CGA
38	a	409	PHO	C2A-CAA-CBA-CGA
38	BD	409	PHO	C2A-CAA-CBA-CGA
23	7	310	CHL	C11-C12-C13-C15
23	AA	310	CHL	C11-C12-C13-C15
23	BQ	601	CHL	C16-C17-C18-C19
24	6	611	CLA	C3-C5-C6-C7
24	B	614	CLA	C3-C5-C6-C7
24	0	611	CLA	C3-C5-C6-C7
24	v	613	CLA	C3-C5-C6-C7
38	R	408	PHO	C3-C5-C6-C7
23	BJ	608	CHL	CBA-CGA-O2A-C1
24	C	512	CLA	CBA-CGA-O2A-C1
24	c	509	CLA	CBA-CGA-O2A-C1
24	BB	304	CLA	CBA-CGA-O2A-C1
24	BJ	613	CLA	CBA-CGA-O2A-C1
24	Ba	305	CLA	CBA-CGA-O2A-C1
24	BF	509	CLA	CBA-CGA-O2A-C1
27	L	102	LHG	C24-C23-O8-C6
27	Az	102	LHG	C24-C23-O8-C6
24	b	606	CLA	C8-C10-C11-C12
24	C	511	CLA	C5-C6-C7-C8
24	BE	606	CLA	C8-C10-C11-C12
34	BF	518	DGD	O1A-C1A-O1G-C1G
24	C	506	CLA	C5-C6-C7-C8
24	BD	410	CLA	C10-C11-C12-C13
26	S	616	NEX	C13-C14-C15-C35
26	Y	318	NEX	C29-C30-C31-C32
26	n	617	NEX	C13-C14-C15-C35
28	G	619	XAT	C13-C14-C15-C35
28	Y	301	XAT	C33-C34-C35-C15
28	Au	619	XAT	C13-C14-C15-C35
30	I	101	LMG	C32-C33-C34-C35
32	d	406	SQD	C10-C11-C12-C13
32	l	102	SQD	C12-C13-C14-C15
30	C	519	LMG	C11-C10-O7-C8
30	c	518	LMG	C11-C10-O7-C8
30	1	519	LMG	C11-C10-O7-C8
30	BF	519	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	1	506	CLA	C5-C6-C7-C8
26	5	617	NEX	C11-C10-C9-C19
26	N	617	NEX	C11-C10-C9-C19
26	N	617	NEX	C20-C13-C14-C15
26	S	616	NEX	C11-C10-C9-C19
26	Y	318	NEX	C20-C13-C14-C15
26	n	617	NEX	C11-C10-C9-C19
26	s	616	NEX	C11-C10-C9-C19
26	y	318	NEX	C20-C13-C14-C15
26	y	318	NEX	C39-C29-C30-C31
26	9	617	NEX	C11-C10-C9-C19
26	A2	617	NEX	C11-C10-C9-C19
26	A2	617	NEX	C20-C13-C14-C15
26	BB	318	NEX	C40-C33-C34-C35
26	BQ	617	NEX	C11-C10-C9-C19
26	BV	616	NEX	C11-C10-C9-C19
26	Ba	318	NEX	C20-C13-C14-C15
26	Ba	318	NEX	C39-C29-C30-C31
28	5	619	XAT	C11-C10-C9-C19
28	N	619	XAT	C11-C10-C9-C19
28	Y	301	XAT	C11-C10-C9-C19
28	n	619	XAT	C11-C10-C9-C19
28	n	619	XAT	C39-C29-C30-C31
28	r	616	XAT	C39-C29-C30-C31
28	9	619	XAT	C11-C10-C9-C19
28	9	619	XAT	C20-C13-C14-C15
28	A2	619	XAT	C11-C10-C9-C19
28	A2	619	XAT	C39-C29-C30-C31
28	BB	301	XAT	C11-C10-C9-C19
28	BQ	619	XAT	C11-C10-C9-C19
28	BQ	619	XAT	C20-C13-C14-C15
28	BQ	619	XAT	C39-C29-C30-C31
28	BU	616	XAT	C39-C29-C30-C31
29	C	515	BCR	C20-C21-C22-C37
29	v	619	BCR	C35-C13-C14-C15
29	BE	618	BCR	C20-C21-C22-C37
29	1	515	BCR	C20-C21-C22-C37
34	1	518	DGD	O6E-C5E-C6E-O5E
24	Ba	311	CLA	C3-C5-C6-C7
23	BQ	607	CHL	C10-C11-C12-C13
27	B	621	LHG	C32-C33-C34-C35
27	L	102	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	c	520	LHG	C26-C27-C28-C29
27	v	621	LHG	C32-C33-C34-C35
27	Az	102	LHG	C9-C10-C11-C12
30	d	405	LMG	C33-C34-C35-C36
30	c	518	LMG	C17-C18-C19-C20
30	Aw	101	LMG	C32-C33-C34-C35
30	BG	405	LMG	C33-C34-C35-C36
30	BF	519	LMG	C17-C18-C19-C20
32	D	406	SQD	C25-C26-C27-C28
32	L	101	SQD	C27-C28-C29-C30
32	BG	406	SQD	C10-C11-C12-C13
32	BG	406	SQD	C25-C26-C27-C28
32	BO	102	SQD	C12-C13-C14-C15
32	R	411	SQD	C29-C30-C31-C32
34	H	102	DGD	CBA-CCA-CDA-CEA
34	H	102	DGD	C3B-C4B-C5B-C6B
34	Av	102	DGD	CBA-CCA-CDA-CEA
34	Av	102	DGD	C3B-C4B-C5B-C6B
34	BK	102	DGD	C9A-CAA-CBA-CCA
34	BF	517	DGD	C5B-C6B-C7B-C8B
34	BF	518	DGD	C3B-C4B-C5B-C6B
24	B	607	CLA	O1A-CGA-O2A-C1
24	v	607	CLA	O1A-CGA-O2A-C1
24	BV	612	CLA	O1A-CGA-O2A-C1
34	C	518	DGD	O1A-C1A-O1G-C1G
24	Au	612	CLA	O1D-CGD-O2D-CED
23	r	605	CHL	C16-C17-C18-C19
23	Au	609	CHL	C11-C12-C13-C15
23	BJ	607	CHL	C16-C17-C18-C20
23	BU	605	CHL	C16-C17-C18-C19
24	6	602	CLA	C11-C12-C13-C14
24	y	311	CLA	C11-C12-C13-C15
24	Ba	311	CLA	C11-C12-C13-C15
23	g	608	CHL	CBA-CGA-O2A-C1
24	C	508	CLA	CBA-CGA-O2A-C1
24	0	611	CLA	CBA-CGA-O2A-C1
24	1	504	CLA	CBA-CGA-O2A-C1
24	1	512	CLA	CBA-CGA-O2A-C1
27	L	102	LHG	C32-C33-C34-C35
27	b	622	LHG	C32-C33-C34-C35
27	c	520	LHG	C12-C13-C14-C15
27	c	520	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	Az	102	LHG	C32-C33-C34-C35
27	BF	521	LHG	C12-C13-C14-C15
27	BF	521	LHG	C26-C27-C28-C29
30	B	620	LMG	C17-C18-C19-C20
30	v	620	LMG	C17-C18-C19-C20
30	BE	621	LMG	C30-C31-C32-C33
32	d	406	SQD	C25-C26-C27-C28
32	2	408	SQD	C11-C12-C13-C14
32	Az	101	SQD	C27-C28-C29-C30
34	C	518	DGD	C4B-C5B-C6B-C7B
34	c	517	DGD	C3B-C4B-C5B-C6B
34	BK	102	DGD	CCA-CDA-CEA-CFA
34	1	518	DGD	C4B-C5B-C6B-C7B
23	7	310	CHL	O1D-CGD-O2D-CED
23	AA	310	CHL	O1D-CGD-O2D-CED
24	6	602	CLA	C10-C11-C12-C13
24	B	608	CLA	C15-C16-C17-C18
24	a	410	CLA	C10-C11-C12-C13
27	L	102	LHG	C7-C8-C9-C10
27	BE	623	LHG	C7-C8-C9-C10
27	BE	624	LHG	C7-C8-C9-C10
30	A0	201	LMG	C10-C11-C12-C13
30	1	501	LMG	C28-C29-C30-C31
27	2	406	LHG	C29-C30-C31-C32
27	BB	319	LHG	C31-C32-C33-C34
27	BE	622	LHG	C32-C33-C34-C35
27	1	521	LHG	C12-C13-C14-C15
27	BF	521	LHG	C31-C32-C33-C34
30	C	501	LMG	C18-C19-C20-C21
30	c	501	LMG	C18-C19-C20-C21
32	L	103	SQD	C11-C12-C13-C14
32	A	413	SQD	C13-C14-C15-C16
32	A	413	SQD	C32-C33-C34-C35
32	2	408	SQD	C29-C30-C31-C32
32	BD	412	SQD	C11-C12-C13-C14
34	h	102	DGD	CCA-CDA-CEA-CFA
24	G	613	CLA	O1A-CGA-O2A-C1
24	Au	613	CLA	O1A-CGA-O2A-C1
34	C	518	DGD	O6E-C5E-C6E-O5E
23	8	307	CHL	C2C-C3C-CAC-CBC
27	b	624	LHG	C32-C33-C34-C35
27	C	521	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
27	BE	624	LHG	C9-C10-C11-C12
27	BE	624	LHG	C30-C31-C32-C33
27	BE	624	LHG	C32-C33-C34-C35
30	B	624	LMG	C32-C33-C34-C35
30	D	405	LMG	C14-C15-C16-C17
30	D	405	LMG	C33-C34-C35-C36
30	b	621	LMG	C17-C18-C19-C20
30	A	412	LMG	C32-C33-C34-C35
30	C	519	LMG	C17-C18-C19-C20
30	v	623	LMG	C32-C33-C34-C35
30	2	407	LMG	C14-C15-C16-C17
30	BE	621	LMG	C17-C18-C19-C20
30	1	501	LMG	C18-C19-C20-C21
32	D	406	SQD	C10-C11-C12-C13
32	D	406	SQD	C29-C30-C31-C32
32	a	412	SQD	C11-C12-C13-C14
32	A1	101	SQD	C11-C12-C13-C14
32	R	411	SQD	C32-C33-C34-C35
34	c	516	DGD	C5B-C6B-C7B-C8B
24	6	613	CLA	O1D-CGD-O2D-CED
24	BD	410	CLA	O1D-CGD-O2D-CED
23	A2	601	CHL	C13-C15-C16-C17
24	S	610	CLA	C5-C6-C7-C8
24	BV	610	CLA	C5-C6-C7-C8
33	F	102	HEM	C3D-CAD-CBD-CGD
33	4	102	HEM	C3D-CAD-CBD-CGD
27	w	201	LHG	C32-C33-C34-C35
27	BQ	618	LHG	C11-C10-C9-C8
27	BY	201	LHG	C32-C33-C34-C35
27	1	521	LHG	C26-C27-C28-C29
30	2	407	LMG	C33-C34-C35-C36
30	A0	201	LMG	C32-C33-C34-C35
30	1	519	LMG	C17-C18-C19-C20
32	l	101	SQD	C11-C12-C13-C14
32	2	408	SQD	C11-C10-C9-C8
32	BO	101	SQD	C11-C12-C13-C14
32	BO	102	SQD	C27-C28-C29-C30
27	Az	102	LHG	C7-C8-C9-C10
30	B	624	LMG	C28-C29-C30-C31
30	v	623	LMG	C28-C29-C30-C31
24	D	401	CLA	O1D-CGD-O2D-CED
26	N	617	NEX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	N	617	NEX	C12-C13-C14-C15
26	Y	318	NEX	C12-C13-C14-C15
26	n	617	NEX	C12-C13-C14-C15
26	s	616	NEX	C11-C10-C9-C8
26	y	318	NEX	C12-C13-C14-C15
26	y	318	NEX	C28-C29-C30-C31
26	9	617	NEX	C11-C10-C9-C8
26	A2	617	NEX	C11-C10-C9-C8
26	A2	617	NEX	C12-C13-C14-C15
26	BB	318	NEX	C32-C33-C34-C35
26	BV	616	NEX	C11-C10-C9-C8
26	Ba	318	NEX	C12-C13-C14-C15
26	Ba	318	NEX	C28-C29-C30-C31
26	Ba	318	NEX	C32-C33-C34-C35
28	5	619	XAT	C11-C10-C9-C8
28	8	312	XAT	C28-C29-C30-C31
28	G	619	XAT	C12-C13-C14-C15
28	N	619	XAT	C12-C13-C14-C15
28	N	619	XAT	C28-C29-C30-C31
28	n	619	XAT	C12-C13-C14-C15
28	n	619	XAT	C28-C29-C30-C31
28	r	616	XAT	C28-C29-C30-C31
28	9	619	XAT	C11-C10-C9-C8
28	9	619	XAT	C32-C33-C34-C35
28	AB	312	XAT	C28-C29-C30-C31
28	Au	619	XAT	C12-C13-C14-C15
28	A2	619	XAT	C12-C13-C14-C15
28	A2	619	XAT	C28-C29-C30-C31
28	BQ	619	XAT	C12-C13-C14-C15
28	BQ	619	XAT	C28-C29-C30-C31
28	BU	616	XAT	C28-C29-C30-C31
29	8	313	BCR	C20-C21-C22-C23
29	f	101	BCR	C12-C13-C14-C15
29	AB	313	BCR	C20-C21-C22-C23
29	BI	101	BCR	C12-C13-C14-C15
29	BF	516	BCR	C20-C21-C22-C23
30	B	624	LMG	C2-C1-O1-C7
30	v	623	LMG	C2-C1-O1-C7
34	h	102	DGD	C2E-C1E-O5D-C6D
34	C	518	DGD	C2E-C1E-O5D-C6D
34	a	401	DGD	C2E-C1E-O5D-C6D
34	a	413	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
34	BK	102	DGD	C2E-C1E-O5D-C6D
34	1	518	DGD	C2E-C1E-O5D-C6D
34	BD	401	DGD	C2E-C1E-O5D-C6D
34	BD	413	DGD	C2E-C1E-O5D-C6D
24	Y	303	CLA	CBA-CGA-O2A-C1
24	Y	304	CLA	CBA-CGA-O2A-C1
24	1	508	CLA	CBA-CGA-O2A-C1
24	BF	513	CLA	CBA-CGA-O2A-C1
27	C	520	LHG	C24-C23-O8-C6
27	1	520	LHG	C24-C23-O8-C6
27	b	624	LHG	C30-C31-C32-C33
27	n	618	LHG	C11-C10-C9-C8
27	BJ	618	LHG	C28-C29-C30-C31
32	L	103	SQD	C9-C10-C11-C12
32	l	102	SQD	C27-C28-C29-C30
32	R	411	SQD	C13-C14-C15-C16
34	Av	102	DGD	CCA-CDA-CEA-CFA
23	Ba	308	CHL	C13-C15-C16-C17
24	B	607	CLA	C8-C10-C11-C12
24	s	610	CLA	C5-C6-C7-C8
24	v	607	CLA	C8-C10-C11-C12
24	BE	615	CLA	C13-C15-C16-C17
24	g	613	CLA	O1A-CGA-O2A-C1
24	y	311	CLA	O1A-CGA-O2A-C1
24	BF	509	CLA	O1A-CGA-O2A-C1
38	R	408	PHO	O1A-CGA-O2A-C1
23	G	609	CHL	C11-C12-C13-C15
23	g	607	CHL	C16-C17-C18-C20
23	g	609	CHL	C11-C12-C13-C15
23	n	601	CHL	C16-C17-C18-C19
23	A2	601	CHL	C16-C17-C18-C19
23	BJ	609	CHL	C11-C12-C13-C15
24	r	603	CLA	C11-C12-C13-C14
24	BU	603	CLA	C11-C12-C13-C14
23	0	601	CHL	O1D-CGD-O2D-CED
24	v	610	CLA	O1D-CGD-O2D-CED
24	c	506	CLA	C4-C3-C5-C6
24	9	603	CLA	C4-C3-C5-C6
31	d	403	PL9	C15-C14-C16-C17
31	BG	403	PL9	C15-C14-C16-C17
27	B	622	LHG	C27-C28-C29-C30
27	b	624	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	C	521	LHG	C12-C13-C14-C15
27	C	521	LHG	C31-C32-C33-C34
27	2	405	LHG	C27-C28-C29-C30
30	B	620	LMG	C19-C20-C21-C22
30	b	621	LMG	C19-C20-C21-C22
30	c	518	LMG	C35-C36-C37-C38
30	v	620	LMG	C19-C20-C21-C22
30	BE	621	LMG	C19-C20-C21-C22
30	BF	501	LMG	C18-C19-C20-C21
32	A	413	SQD	C11-C12-C13-C14
32	A	413	SQD	C31-C32-C33-C34
32	A1	101	SQD	C9-C10-C11-C12
32	BO	101	SQD	C9-C10-C11-C12
32	R	411	SQD	C33-C34-C35-C36
34	H	102	DGD	CCA-CDA-CEA-CFA
34	h	102	DGD	CBA-CCA-CDA-CEA
34	C	517	DGD	C3B-C4B-C5B-C6B
34	1	517	DGD	C3B-C4B-C5B-C6B
24	B	606	CLA	C11-C12-C13-C14
24	I	102	CLA	C6-C7-C8-C9
24	b	609	CLA	C6-C7-C8-C9
24	y	313	CLA	C11-C10-C8-C9
24	C	504	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	c	507	CLA	C14-C13-C15-C16
24	v	606	CLA	C11-C12-C13-C14
24	Aw	102	CLA	C6-C7-C8-C9
24	A2	603	CLA	C11-C10-C8-C9
24	A6	602	CLA	C6-C7-C8-C9
24	BB	303	CLA	C6-C7-C8-C9
24	BE	609	CLA	C6-C7-C8-C9
24	Ba	313	CLA	C11-C10-C8-C9
24	1	504	CLA	C14-C13-C15-C16
24	1	506	CLA	C14-C13-C15-C16
24	1	511	CLA	C11-C12-C13-C14
24	BF	507	CLA	C14-C13-C15-C16
23	y	308	CHL	O1D-CGD-O2D-CED
23	BU	607	CHL	O1D-CGD-O2D-CED
24	a	410	CLA	O1D-CGD-O2D-CED
38	a	409	PHO	O1D-CGD-O2D-CED
38	BD	409	PHO	O1D-CGD-O2D-CED
24	R	405	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	A	412	LMG	C10-C11-C12-C13
30	C	501	LMG	C28-C29-C30-C31
27	L	102	LHG	C30-C31-C32-C33
27	W	201	LHG	C32-C33-C34-C35
27	Az	102	LHG	C30-C31-C32-C33
27	A0	202	LHG	C32-C33-C34-C35
27	1	521	LHG	C31-C32-C33-C34
30	D	405	LMG	C18-C19-C20-C21
30	I	101	LMG	C30-C31-C32-C33
30	c	518	LMG	C11-C12-C13-C14
30	2	407	LMG	C18-C19-C20-C21
30	1	519	LMG	C11-C12-C13-C14
30	BF	519	LMG	C11-C12-C13-C14
30	BF	519	LMG	C35-C36-C37-C38
32	d	406	SQD	C29-C30-C31-C32
32	l	101	SQD	C9-C10-C11-C12
32	A	413	SQD	C29-C30-C31-C32
32	a	412	SQD	C31-C32-C33-C34
32	BG	406	SQD	C11-C12-C13-C14
32	BG	406	SQD	C29-C30-C31-C32
32	R	411	SQD	C11-C12-C13-C14
32	R	411	SQD	C31-C32-C33-C34
32	BD	412	SQD	C31-C32-C33-C34
34	C	516	DGD	C4B-C5B-C6B-C7B
34	C	516	DGD	C5B-C6B-C7B-C8B
34	a	413	DGD	C4B-C5B-C6B-C7B
34	1	516	DGD	C4B-C5B-C6B-C7B
34	BD	413	DGD	C4B-C5B-C6B-C7B
24	B	605	CLA	C8-C10-C11-C12
24	c	511	CLA	C15-C16-C17-C18
24	A2	603	CLA	C10-C11-C12-C13
24	1	511	CLA	C5-C6-C7-C8
34	Av	102	DGD	O6E-C5E-C6E-O5E
23	8	305	CHL	C2A-CAA-CBA-CGA
23	G	605	CHL	C2A-CAA-CBA-CGA
23	y	310	CHL	C2A-CAA-CBA-CGA
23	0	605	CHL	C2A-CAA-CBA-CGA
23	Au	605	CHL	C2A-CAA-CBA-CGA
24	5	604	CLA	C2A-CAA-CBA-CGA
24	D	402	CLA	C2A-CAA-CBA-CGA
24	Y	315	CLA	C2A-CAA-CBA-CGA
24	y	315	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C2A-CAA-CBA-CGA
24	r	608	CLA	C2A-CAA-CBA-CGA
24	9	602	CLA	C2A-CAA-CBA-CGA
24	9	604	CLA	C2A-CAA-CBA-CGA
24	9	610	CLA	C2A-CAA-CBA-CGA
24	2	403	CLA	C2A-CAA-CBA-CGA
24	A2	611	CLA	C2A-CAA-CBA-CGA
24	BG	402	CLA	C2A-CAA-CBA-CGA
24	Ba	315	CLA	C2A-CAA-CBA-CGA
24	BU	608	CLA	C2A-CAA-CBA-CGA
38	A	409	PHO	O1A-CGA-O2A-C1
25	Ba	316	LUT	C7-C8-C9-C19
26	5	617	NEX	C11-C12-C13-C20
26	g	617	NEX	C11-C12-C13-C20
28	5	619	XAT	C11-C12-C13-C20
28	5	619	XAT	C27-C28-C29-C39
28	7	301	XAT	C11-C12-C13-C20
28	7	318	XAT	C11-C12-C13-C20
28	y	301	XAT	C11-C12-C13-C20
28	r	616	XAT	C31-C32-C33-C40
28	9	619	XAT	C27-C28-C29-C39
28	AA	301	XAT	C11-C12-C13-C20
28	AA	318	XAT	C11-C12-C13-C20
28	BU	616	XAT	C31-C32-C33-C40
29	B	623	BCR	C7-C8-C9-C34
29	k	101	BCR	C7-C8-C9-C34
29	v	622	BCR	C7-C8-C9-C34
27	d	404	LHG	C29-C30-C31-C32
30	C	519	LMG	C11-C12-C13-C14
30	C	519	LMG	C12-C13-C14-C15
30	C	519	LMG	C31-C32-C33-C34
30	1	519	LMG	C12-C13-C14-C15
30	1	519	LMG	C31-C32-C33-C34
32	D	406	SQD	C9-C10-C11-C12
32	A	413	SQD	C33-C34-C35-C36
32	2	408	SQD	C18-C19-C20-C21
34	1	517	DGD	C4A-C5A-C6A-C7A
27	B	622	LHG	O1-C1-C2-C3
27	b	623	LHG	O1-C1-C2-C3
27	C	521	LHG	O1-C1-C2-C3
27	c	520	LHG	O1-C1-C2-C3
27	BQ	618	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	1	521	LHG	O1-C1-C2-C3
27	BF	521	LHG	O1-C1-C2-C3
26	5	617	NEX	C31-C32-C33-C34
26	7	319	NEX	C31-C32-C33-C34
26	AA	319	NEX	C11-C12-C13-C14
26	AA	319	NEX	C31-C32-C33-C34
26	Au	617	NEX	C11-C12-C13-C14
28	7	301	XAT	C31-C32-C33-C34
28	n	619	XAT	C31-C32-C33-C34
24	BF	507	CLA	C3-C5-C6-C7
38	a	409	PHO	C3-C5-C6-C7
23	G	601	CHL	C13-C15-C16-C17
23	Au	608	CHL	C15-C16-C17-C18
24	7	303	CLA	C5-C6-C7-C8
24	b	608	CLA	C5-C6-C7-C8
24	v	608	CLA	C15-C16-C17-C18
34	a	401	DGD	C2B-C1B-O2G-C2G
34	BD	401	DGD	C2B-C1B-O2G-C2G
27	B	621	LHG	C28-C29-C30-C31
27	b	622	LHG	C27-C28-C29-C30
27	v	621	LHG	C28-C29-C30-C31
27	BG	404	LHG	C29-C30-C31-C32
30	B	624	LMG	C37-C38-C39-C40
30	v	623	LMG	C37-C38-C39-C40
30	Aw	101	LMG	C30-C31-C32-C33
32	L	101	SQD	C12-C13-C14-C15
32	2	408	SQD	C10-C11-C12-C13
34	C	517	DGD	C4A-C5A-C6A-C7A
23	Y	308	CHL	CBD-CGD-O2D-CED
27	b	624	LHG	C7-C8-C9-C10
34	BK	102	DGD	C1B-C2B-C3B-C4B
23	Ba	308	CHL	O1D-CGD-O2D-CED
27	b	623	LHG	C27-C28-C29-C30
27	Az	102	LHG	C10-C11-C12-C13
27	Az	102	LHG	C31-C32-C33-C34
27	BE	622	LHG	C27-C28-C29-C30
30	B	620	LMG	C13-C14-C15-C16
30	b	621	LMG	C13-C14-C15-C16
30	b	621	LMG	C30-C31-C32-C33
30	C	501	LMG	C32-C33-C34-C35
30	c	518	LMG	C31-C32-C33-C34
30	v	620	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	1	501	LMG	C32-C33-C34-C35
30	BF	519	LMG	C31-C32-C33-C34
32	A	413	SQD	C25-C26-C27-C28
34	c	516	DGD	C4B-C5B-C6B-C7B
34	c	517	DGD	C4A-C5A-C6A-C7A
34	BD	401	DGD	C5B-C6B-C7B-C8B
34	BF	517	DGD	C4B-C5B-C6B-C7B
34	BF	518	DGD	C4A-C5A-C6A-C7A
34	H	102	DGD	O6E-C5E-C6E-O5E
34	h	102	DGD	O6E-C5E-C6E-O5E
24	c	509	CLA	O1A-CGA-O2A-C1
23	7	308	CHL	C4B-C3B-CAB-CBB
23	AA	308	CHL	C4B-C3B-CAB-CBB
23	Ba	308	CHL	C4B-C3B-CAB-CBB
24	5	610	CLA	C4B-C3B-CAB-CBB
24	6	611	CLA	C4B-C3B-CAB-CBB
24	7	312	CLA	C4B-C3B-CAB-CBB
24	N	603	CLA	C4B-C3B-CAB-CBB
24	N	611	CLA	C4B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
24	C	511	CLA	C4B-C3B-CAB-CBB
24	c	507	CLA	C4B-C3B-CAB-CBB
24	0	611	CLA	C4B-C3B-CAB-CBB
24	AA	312	CLA	C4B-C3B-CAB-CBB
24	A2	611	CLA	C4B-C3B-CAB-CBB
24	BV	608	CLA	C4B-C3B-CAB-CBB
24	1	506	CLA	C4B-C3B-CAB-CBB
24	BF	507	CLA	C4B-C3B-CAB-CBB
23	Y	308	CHL	C16-C17-C18-C19
23	Y	310	CHL	C16-C17-C18-C20
23	r	605	CHL	C16-C17-C18-C20
23	r	607	CHL	C11-C12-C13-C15
23	A2	601	CHL	C16-C17-C18-C20
23	BQ	601	CHL	C16-C17-C18-C20
23	BU	605	CHL	C16-C17-C18-C20
24	6	602	CLA	C11-C12-C13-C15
24	b	605	CLA	C16-C17-C18-C20
24	0	602	CLA	C11-C12-C13-C14
24	BE	605	CLA	C16-C17-C18-C20
34	C	518	DGD	O6E-C1E-O5D-C6D
34	a	401	DGD	O6E-C1E-O5D-C6D
34	a	413	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
34	1	518	DGD	O6E-C1E-O5D-C6D
34	BD	401	DGD	O6E-C1E-O5D-C6D
34	BD	413	DGD	O6E-C1E-O5D-C6D
23	G	608	CHL	C15-C16-C17-C18
23	Y	308	CHL	C13-C15-C16-C17
23	Au	601	CHL	C13-C15-C16-C17
23	BQ	607	CHL	C13-C15-C16-C17
24	N	603	CLA	C10-C11-C12-C13
24	b	615	CLA	C13-C15-C16-C17
24	C	513	CLA	C13-C15-C16-C17
24	BF	505	CLA	C13-C15-C16-C17
23	g	607	CHL	O1D-CGD-O2D-CED
27	L	102	LHG	C10-C11-C12-C13
27	L	102	LHG	C31-C32-C33-C34
27	Y	319	LHG	C31-C32-C33-C34
27	b	624	LHG	C31-C32-C33-C34
27	BE	624	LHG	C31-C32-C33-C34
27	BG	404	LHG	C30-C31-C32-C33
30	B	620	LMG	C18-C19-C20-C21
30	d	405	LMG	C18-C19-C20-C21
30	i	101	LMG	C32-C33-C34-C35
30	C	519	LMG	C16-C17-C18-C19
30	c	518	LMG	C12-C13-C14-C15
30	v	620	LMG	C13-C14-C15-C16
30	BE	621	LMG	C13-C14-C15-C16
30	BG	405	LMG	C18-C19-C20-C21
30	BL	101	LMG	C32-C33-C34-C35
30	1	519	LMG	C16-C17-C18-C19
30	BF	519	LMG	C12-C13-C14-C15
32	D	406	SQD	C18-C19-C20-C21
32	d	406	SQD	C9-C10-C11-C12
32	a	412	SQD	C33-C34-C35-C36
32	Az	101	SQD	C12-C13-C14-C15
32	R	411	SQD	C25-C26-C27-C28
32	BD	412	SQD	C33-C34-C35-C36
34	h	102	DGD	C5B-C6B-C7B-C8B
34	C	518	DGD	C2A-C3A-C4A-C5A
34	a	401	DGD	C5B-C6B-C7B-C8B
34	BK	102	DGD	C5B-C6B-C7B-C8B
34	1	516	DGD	C5B-C6B-C7B-C8B
23	6	601	CHL	O1D-CGD-O2D-CED
27	G	618	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	G	618	LHG	C25-C26-C27-C28
27	g	618	LHG	C28-C29-C30-C31
27	BE	623	LHG	C27-C28-C29-C30
30	v	623	LMG	C30-C31-C32-C33
32	2	408	SQD	C9-C10-C11-C12
32	BG	406	SQD	C9-C10-C11-C12
34	1	518	DGD	C2A-C3A-C4A-C5A
27	b	623	LHG	C7-C8-C9-C10
23	n	607	CHL	C13-C15-C16-C17
23	A2	607	CHL	C13-C15-C16-C17
24	1	513	CLA	C13-C15-C16-C17
24	BF	511	CLA	C15-C16-C17-C18
24	BJ	613	CLA	O1A-CGA-O2A-C1
24	Ba	305	CLA	O1A-CGA-O2A-C1
24	BU	611	CLA	O1A-CGA-O2A-C1
30	B	624	LMG	C30-C31-C32-C33
30	c	501	LMG	C32-C33-C34-C35
30	c	518	LMG	C32-C33-C34-C35
32	a	412	SQD	C25-C26-C27-C28
32	BD	412	SQD	C25-C26-C27-C28
34	c	517	DGD	C6B-C7B-C8B-C9B
34	1	518	DGD	CCA-CDA-CEA-CFA
24	7	311	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
24	9	603	CLA	CBA-CGA-O2A-C1
24	AA	311	CLA	CBA-CGA-O2A-C1
27	b	624	LHG	C24-C23-O8-C6
30	i	101	LMG	C29-C28-O8-C9
30	BL	101	LMG	C29-C28-O8-C9
23	g	607	CHL	C4C-C3C-CAC-CBC
27	B	622	LHG	C32-C33-C34-C35
27	C	521	LHG	C24-C25-C26-C27
27	c	520	LHG	C14-C15-C16-C17
27	Au	618	LHG	C18-C19-C20-C21
27	Au	618	LHG	C25-C26-C27-C28
27	BJ	618	LHG	C25-C26-C27-C28
30	BF	501	LMG	C32-C33-C34-C35
32	D	406	SQD	C11-C12-C13-C14
23	Au	605	CHL	O1D-CGD-O2D-CED
23	BJ	607	CHL	O1D-CGD-O2D-CED
23	BQ	607	CHL	O1D-CGD-O2D-CED
24	B	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	Y	303	CLA	O1D-CGD-O2D-CED
23	5	605	CHL	C3A-C2A-CAA-CBA
23	N	601	CHL	C3A-C2A-CAA-CBA
23	N	608	CHL	C3A-C2A-CAA-CBA
23	n	608	CHL	C3A-C2A-CAA-CBA
23	9	605	CHL	C3A-C2A-CAA-CBA
23	A2	601	CHL	C3A-C2A-CAA-CBA
23	A2	608	CHL	C3A-C2A-CAA-CBA
23	BB	308	CHL	C3A-C2A-CAA-CBA
23	BQ	608	CHL	C3A-C2A-CAA-CBA
24	6	611	CLA	C3A-C2A-CAA-CBA
24	7	314	CLA	C3A-C2A-CAA-CBA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	N	610	CLA	C3A-C2A-CAA-CBA
24	N	614	CLA	C3A-C2A-CAA-CBA
24	n	611	CLA	C3A-C2A-CAA-CBA
24	n	614	CLA	C3A-C2A-CAA-CBA
24	r	604	CLA	C3A-C2A-CAA-CBA
24	0	611	CLA	C3A-C2A-CAA-CBA
24	AA	314	CLA	C3A-C2A-CAA-CBA
24	v	608	CLA	C3A-C2A-CAA-CBA
24	BQ	610	CLA	C3A-C2A-CAA-CBA
24	BQ	611	CLA	C3A-C2A-CAA-CBA
24	BQ	614	CLA	C3A-C2A-CAA-CBA
24	BU	604	CLA	C3A-C2A-CAA-CBA
23	BB	308	CHL	C13-C15-C16-C17
24	c	505	CLA	C13-C15-C16-C17
24	BE	608	CLA	C5-C6-C7-C8
27	g	618	LHG	C25-C26-C27-C28
27	n	618	LHG	C25-C26-C27-C28
27	c	520	LHG	C24-C25-C26-C27
27	2	405	LHG	C32-C33-C34-C35
27	BQ	618	LHG	C25-C26-C27-C28
30	BF	519	LMG	C32-C33-C34-C35
32	D	406	SQD	C11-C10-C9-C8
32	A	413	SQD	C16-C17-C18-C19
32	2	408	SQD	C25-C26-C27-C28
34	h	102	DGD	C9A-CAA-CBA-CCA
34	C	518	DGD	CCA-CDA-CEA-CFA
34	BK	102	DGD	CBA-CCA-CDA-CEA
27	1	521	LHG	C7-C8-C9-C10
23	G	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	y	302	CHL	O1D-CGD-O2D-CED
23	BB	302	CHL	O1D-CGD-O2D-CED
24	v	615	CLA	O1D-CGD-O2D-CED
24	2	402	CLA	O1D-CGD-O2D-CED
24	r	611	CLA	O1A-CGA-O2A-C1
34	C	517	DGD	O1A-C1A-O1G-C1G
23	7	310	CHL	C11-C12-C13-C14
23	G	607	CHL	C16-C17-C18-C20
23	N	601	CHL	C16-C17-C18-C19
23	N	601	CHL	C16-C17-C18-C20
23	g	609	CHL	C11-C12-C13-C14
23	n	607	CHL	C16-C17-C18-C19
23	r	607	CHL	C11-C12-C13-C14
23	AA	310	CHL	C11-C12-C13-C14
23	BB	310	CHL	C16-C17-C18-C20
23	BJ	609	CHL	C11-C12-C13-C14
23	BQ	607	CHL	C16-C17-C18-C19
23	BU	607	CHL	C11-C12-C13-C14
23	BU	607	CHL	C11-C12-C13-C15
24	b	605	CLA	C16-C17-C18-C19
24	r	603	CLA	C11-C12-C13-C15
24	0	602	CLA	C11-C12-C13-C15
24	BE	605	CLA	C16-C17-C18-C19
24	BU	603	CLA	C11-C12-C13-C15
23	9	609	CHL	C2C-C3C-CAC-CBC
27	d	404	LHG	C30-C31-C32-C33
27	Az	102	LHG	C29-C30-C31-C32
27	1	521	LHG	C24-C25-C26-C27
27	BF	521	LHG	C14-C15-C16-C17
27	BF	521	LHG	C24-C25-C26-C27
30	c	518	LMG	C16-C17-C18-C19
30	BG	405	LMG	C16-C17-C18-C19
34	BD	401	DGD	C6A-C7A-C8A-C9A
30	A	412	LMG	O6-C5-C6-O5
34	BK	102	DGD	O6E-C5E-C6E-O5E
23	BB	308	CHL	CBD-CGD-O2D-CED
24	G	610	CLA	C15-C16-C17-C18
27	L	102	LHG	C29-C30-C31-C32
30	v	620	LMG	C32-C33-C34-C35
30	v	620	LMG	C34-C35-C36-C37
30	BF	501	LMG	C17-C18-C19-C20
34	a	401	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
34	a	401	DGD	O6D-C5D-C6D-O5D
34	BD	401	DGD	O6D-C5D-C6D-O5D
26	Y	318	NEX	C14-C15-C35-C34
28	r	616	XAT	C14-C15-C35-C34
28	BU	616	XAT	C14-C15-C35-C34
24	c	507	CLA	C3-C5-C6-C7
24	v	615	CLA	C3-C5-C6-C7
27	C	521	LHG	C7-C8-C9-C10
32	R	411	SQD	C16-C17-C18-C19
24	C	504	CLA	O1A-CGA-O2A-C1
24	C	512	CLA	O1A-CGA-O2A-C1
23	N	607	CHL	C13-C15-C16-C17
23	Ba	310	CHL	C15-C16-C17-C18
24	5	603	CLA	C4-C3-C5-C6
24	b	616	CLA	C4-C3-C5-C6
31	d	403	PL9	C30-C29-C31-C32
24	c	504	CLA	CBA-CGA-O2A-C1
24	5	603	CLA	C2-C3-C5-C6
24	b	616	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6
24	BE	616	CLA	C2-C3-C5-C6
31	d	403	PL9	C13-C14-C16-C17
31	BG	403	PL9	C13-C14-C16-C17
27	B	621	LHG	C8-C7-O7-C5
27	v	621	LHG	C8-C7-O7-C5
34	C	518	DGD	C2B-C1B-O2G-C2G
34	1	518	DGD	C2B-C1B-O2G-C2G
27	c	519	LHG	C27-C28-C29-C30
27	Az	102	LHG	C27-C28-C29-C30
30	B	620	LMG	C32-C33-C34-C35
30	d	405	LMG	C16-C17-C18-C19
34	BF	518	DGD	C6B-C7B-C8B-C9B
23	Y	302	CHL	O1D-CGD-O2D-CED
23	Ba	302	CHL	O1D-CGD-O2D-CED
23	6	605	CHL	C2A-CAA-CBA-CGA
27	5	618	LHG	O1-C1-C2-O2
27	B	622	LHG	O1-C1-C2-O2
27	b	622	LHG	O1-C1-C2-O2
27	9	618	LHG	O1-C1-C2-O2
27	BE	622	LHG	O1-C1-C2-O2
27	BE	624	LHG	O1-C1-C2-O2
24	Au	610	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	L	102	LHG	C27-C28-C29-C30
27	2	406	LHG	C11-C10-C9-C8
27	BE	623	LHG	C30-C31-C32-C33
27	BF	520	LHG	C27-C28-C29-C30
30	B	620	LMG	C34-C35-C36-C37
30	B	624	LMG	C34-C35-C36-C37
30	v	623	LMG	C34-C35-C36-C37
30	BF	519	LMG	C16-C17-C18-C19
32	a	412	SQD	C28-C29-C30-C31
32	a	412	SQD	C32-C33-C34-C35
32	BD	412	SQD	C32-C33-C34-C35
34	C	517	DGD	C6B-C7B-C8B-C9B
34	C	518	DGD	C6A-C7A-C8A-C9A
34	Av	102	DGD	C9A-CAA-CBA-CCA
34	1	518	DGD	C6A-C7A-C8A-C9A
34	BD	413	DGD	C2A-C3A-C4A-C5A
23	N	607	CHL	C10-C11-C12-C13
23	9	607	CHL	C10-C11-C12-C13
23	n	607	CHL	O1D-CGD-O2D-CED
34	1	517	DGD	O1A-C1A-O1G-C1G
23	BB	308	CHL	C16-C17-C18-C19
23	Ba	308	CHL	C16-C17-C18-C19
24	Y	311	CLA	C11-C12-C13-C15
23	5	609	CHL	C2C-C3C-CAC-CBC
23	Ba	308	CHL	C4C-C3C-CAC-CBC
32	d	406	SQD	C11-C12-C13-C14
23	7	308	CHL	C2B-C3B-CAB-CBB
23	y	308	CHL	C2B-C3B-CAB-CBB
23	AA	308	CHL	C2B-C3B-CAB-CBB
23	Ba	308	CHL	C2B-C3B-CAB-CBB
24	5	610	CLA	C2B-C3B-CAB-CBB
24	6	611	CLA	C2B-C3B-CAB-CBB
24	7	312	CLA	C2B-C3B-CAB-CBB
24	G	611	CLA	C2B-C3B-CAB-CBB
24	N	603	CLA	C2B-C3B-CAB-CBB
24	N	611	CLA	C2B-C3B-CAB-CBB
24	s	608	CLA	C2B-C3B-CAB-CBB
24	C	506	CLA	C2B-C3B-CAB-CBB
24	C	511	CLA	C2B-C3B-CAB-CBB
24	c	507	CLA	C2B-C3B-CAB-CBB
24	9	604	CLA	C2B-C3B-CAB-CBB
24	AA	312	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	Au	611	CLA	C2B-C3B-CAB-CBB
24	A2	611	CLA	C2B-C3B-CAB-CBB
24	BV	608	CLA	C2B-C3B-CAB-CBB
24	1	506	CLA	C2B-C3B-CAB-CBB
24	BF	507	CLA	C2B-C3B-CAB-CBB
23	y	310	CHL	C15-C16-C17-C18
24	B	615	CLA	C8-C10-C11-C12
23	Ba	310	CHL	C4C-C3C-CAC-CBC
27	D	404	LHG	C11-C10-C9-C8
32	R	411	SQD	C28-C29-C30-C31
32	BD	412	SQD	C28-C29-C30-C31
34	a	413	DGD	C2A-C3A-C4A-C5A
24	c	514	CLA	C3-C5-C6-C7
34	a	401	DGD	C4D-C5D-C6D-O5D
34	BD	401	DGD	C4D-C5D-C6D-O5D
27	W	201	LHG	C24-C23-O8-C6
27	b	623	LHG	C30-C31-C32-C33
32	A	413	SQD	C28-C29-C30-C31
32	2	408	SQD	C27-C28-C29-C30
23	g	608	CHL	O1A-CGA-O2A-C1
23	BJ	608	CHL	O1A-CGA-O2A-C1
24	6	611	CLA	O1A-CGA-O2A-C1
27	b	624	LHG	C27-C28-C29-C30
27	BF	521	LHG	C32-C33-C34-C35
30	D	405	LMG	C32-C33-C34-C35
30	b	621	LMG	C34-C35-C36-C37
30	C	519	LMG	C35-C36-C37-C38
30	BE	621	LMG	C18-C19-C20-C21
32	BD	412	SQD	C16-C17-C18-C19
30	B	624	LMG	O9-C10-O7-C8
30	v	623	LMG	O9-C10-O7-C8
31	BG	403	PL9	C47-C48-C49-C50
23	y	308	CHL	C2C-C3C-CAC-CBC
27	BE	624	LHG	C27-C28-C29-C30
27	BG	404	LHG	C10-C11-C12-C13
27	1	521	LHG	C32-C33-C34-C35
32	a	412	SQD	C13-C14-C15-C16
32	BD	412	SQD	C13-C14-C15-C16
34	H	102	DGD	C9A-CAA-CBA-CCA
24	b	609	CLA	C8-C10-C11-C12
24	v	605	CLA	C8-C10-C11-C12
24	Y	304	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	C	508	CLA	O1A-CGA-O2A-C1
24	0	611	CLA	O1A-CGA-O2A-C1
24	BB	304	CLA	O1A-CGA-O2A-C1
24	1	504	CLA	O1A-CGA-O2A-C1
24	1	512	CLA	O1A-CGA-O2A-C1
24	BF	513	CLA	O1A-CGA-O2A-C1
34	a	413	DGD	O1A-C1A-O1G-C1G
34	BD	413	DGD	O1A-C1A-O1G-C1G
27	B	621	LHG	C27-C28-C29-C30
27	G	618	LHG	C27-C28-C29-C30
27	d	404	LHG	C11-C10-C9-C8
27	c	520	LHG	C32-C33-C34-C35
30	b	621	LMG	C18-C19-C20-C21
30	C	519	LMG	C32-C33-C34-C35
32	a	412	SQD	C16-C17-C18-C19
34	1	517	DGD	C6B-C7B-C8B-C9B
23	n	601	CHL	C16-C17-C18-C20
23	y	308	CHL	C16-C17-C18-C19
23	A2	607	CHL	C16-C17-C18-C19
24	BF	514	CLA	C3-C5-C6-C7
25	5	615	LUT	C1-C6-C7-C8
25	5	616	LUT	C1-C6-C7-C8
25	5	616	LUT	C5-C6-C7-C8
25	G	616	LUT	C1-C6-C7-C8
25	N	616	LUT	C1-C6-C7-C8
25	Au	616	LUT	C1-C6-C7-C8
29	8	313	BCR	C5-C6-C7-C8
29	B	617	BCR	C1-C6-C7-C8
29	B	617	BCR	C5-C6-C7-C8
29	B	619	BCR	C1-C6-C7-C8
29	B	619	BCR	C5-C6-C7-C8
29	F	101	BCR	C1-C6-C7-C8
29	F	101	BCR	C5-C6-C7-C8
29	H	101	BCR	C5-C6-C7-C8
29	H	101	BCR	C23-C24-C25-C26
29	H	101	BCR	C23-C24-C25-C30
29	K	101	BCR	C5-C6-C7-C8
29	K	102	BCR	C1-C6-C7-C8
29	K	102	BCR	C5-C6-C7-C8
29	K	102	BCR	C23-C24-C25-C26
29	K	102	BCR	C23-C24-C25-C30
29	b	618	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	b	618	BCR	C5-C6-C7-C8
29	b	620	BCR	C1-C6-C7-C8
29	b	620	BCR	C5-C6-C7-C8
29	b	620	BCR	C23-C24-C25-C26
29	b	620	BCR	C23-C24-C25-C30
29	f	101	BCR	C1-C6-C7-C8
29	f	101	BCR	C5-C6-C7-C8
29	h	101	BCR	C23-C24-C25-C26
29	h	101	BCR	C23-C24-C25-C30
29	k	101	BCR	C5-C6-C7-C8
29	z	101	BCR	C1-C6-C7-C8
29	z	101	BCR	C5-C6-C7-C8
29	z	102	BCR	C5-C6-C7-C8
29	z	102	BCR	C23-C24-C25-C26
29	z	102	BCR	C23-C24-C25-C30
29	C	514	BCR	C1-C6-C7-C8
29	C	514	BCR	C5-C6-C7-C8
29	a	411	BCR	C23-C24-C25-C26
29	AB	313	BCR	C5-C6-C7-C8
29	v	617	BCR	C1-C6-C7-C8
29	v	617	BCR	C5-C6-C7-C8
29	v	619	BCR	C1-C6-C7-C8
29	v	619	BCR	C5-C6-C7-C8
29	4	101	BCR	C1-C6-C7-C8
29	4	101	BCR	C5-C6-C7-C8
29	Av	101	BCR	C1-C6-C7-C8
29	Av	101	BCR	C5-C6-C7-C8
29	Av	101	BCR	C23-C24-C25-C26
29	Av	101	BCR	C23-C24-C25-C30
29	Ay	101	BCR	C1-C6-C7-C8
29	Ay	101	BCR	C5-C6-C7-C8
29	Ay	102	BCR	C5-C6-C7-C8
29	Ay	102	BCR	C23-C24-C25-C26
29	Ay	102	BCR	C23-C24-C25-C30
29	BE	618	BCR	C1-C6-C7-C8
29	BE	618	BCR	C5-C6-C7-C8
29	BE	620	BCR	C1-C6-C7-C8
29	BE	620	BCR	C5-C6-C7-C8
29	BE	620	BCR	C23-C24-C25-C26
29	BE	620	BCR	C23-C24-C25-C30
29	BI	101	BCR	C1-C6-C7-C8
29	BI	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	BK	101	BCR	C23-C24-C25-C26
29	BK	101	BCR	C23-C24-C25-C30
29	BN	101	BCR	C5-C6-C7-C8
29	Bb	101	BCR	C23-C24-C25-C26
29	Bb	101	BCR	C23-C24-C25-C30
29	1	514	BCR	C5-C6-C7-C8
29	BF	515	BCR	C1-C6-C7-C8
29	BF	515	BCR	C5-C6-C7-C8
29	BF	516	BCR	C23-C24-C25-C26
23	5	607	CHL	C10-C11-C12-C13
23	A2	607	CHL	C10-C11-C12-C13
30	A0	201	LMG	O6-C5-C6-O5
27	b	622	LHG	C28-C29-C30-C31
27	BE	622	LHG	C28-C29-C30-C31
30	c	501	LMG	C17-C18-C19-C20
30	2	407	LMG	C32-C33-C34-C35
30	BE	621	LMG	C34-C35-C36-C37
30	1	519	LMG	C32-C33-C34-C35
24	y	313	CLA	O1D-CGD-O2D-CED
24	5	603	CLA	CBA-CGA-O2A-C1
24	S	610	CLA	CBA-CGA-O2A-C1
24	Y	314	CLA	CBA-CGA-O2A-C1
24	y	305	CLA	CBA-CGA-O2A-C1
24	9	604	CLA	CBA-CGA-O2A-C1
24	A6	610	CLA	CBA-CGA-O2A-C1
24	BF	504	CLA	CBA-CGA-O2A-C1
27	A0	202	LHG	C24-C23-O8-C6
30	BE	621	LMG	C29-C28-O8-C9
23	G	601	CHL	C15-C16-C17-C18
23	Y	310	CHL	C15-C16-C17-C18
24	7	304	CLA	C5-C6-C7-C8
24	Y	313	CLA	C10-C11-C12-C13
24	b	607	CLA	C13-C15-C16-C17
24	s	602	CLA	C5-C6-C7-C8
24	C	506	CLA	C13-C15-C16-C17
24	AA	304	CLA	C5-C6-C7-C8
24	A2	613	CLA	C8-C10-C11-C12
24	BB	313	CLA	C10-C11-C12-C13
24	BE	607	CLA	C13-C15-C16-C17
24	1	506	CLA	C13-C15-C16-C17
27	N	618	LHG	C24-C25-C26-C27
27	C	520	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	C	521	LHG	C32-C33-C34-C35
27	v	621	LHG	C27-C28-C29-C30
27	A2	618	LHG	C24-C25-C26-C27
27	BE	624	LHG	C29-C30-C31-C32
30	c	501	LMG	C34-C35-C36-C37
30	v	620	LMG	C33-C34-C35-C36
30	2	407	LMG	C12-C13-C14-C15
30	Aw	101	LMG	C36-C37-C38-C39
34	a	413	DGD	C6A-C7A-C8A-C9A
34	BK	102	DGD	C9B-CAB-CBB-CCB
34	1	518	DGD	C5A-C6A-C7A-C8A
34	BD	413	DGD	C6A-C7A-C8A-C9A
24	6	614	CLA	O2A-C1-C2-C3
24	0	614	CLA	O2A-C1-C2-C3
24	Y	303	CLA	O1A-CGA-O2A-C1
24	c	513	CLA	O1A-CGA-O2A-C1
24	1	508	CLA	O1A-CGA-O2A-C1
23	5	609	CHL	C14-C13-C15-C16
23	9	609	CHL	C14-C13-C15-C16
27	B	622	LHG	C7-C8-C9-C10
34	a	413	DGD	C1A-C2A-C3A-C4A
27	Au	618	LHG	C27-C28-C29-C30
27	A2	618	LHG	C33-C34-C35-C36
30	I	101	LMG	C36-C37-C38-C39
30	b	621	LMG	C32-C33-C34-C35
23	Au	601	CHL	C15-C16-C17-C18
23	BB	310	CHL	C15-C16-C17-C18
24	C	510	CLA	C15-C16-C17-C18
38	R	408	PHO	C8-C10-C11-C12
23	BJ	607	CHL	C4C-C3C-CAC-CBC
27	b	624	LHG	C29-C30-C31-C32
27	g	618	LHG	C18-C19-C20-C21
27	1	520	LHG	C27-C28-C29-C30
30	1	519	LMG	C35-C36-C37-C38
32	A1	101	SQD	C31-C32-C33-C34
32	BG	406	SQD	C11-C10-C9-C8
34	C	518	DGD	C5A-C6A-C7A-C8A
23	G	607	CHL	C4-C3-C5-C6
23	y	302	CHL	C4-C3-C5-C6
23	Au	607	CHL	C4-C3-C5-C6
23	BJ	607	CHL	C4-C3-C5-C6
24	I	102	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	y	313	CLA	C4-C3-C5-C6
24	Ba	313	CLA	C4-C3-C5-C6
24	BF	506	CLA	C4-C3-C5-C6
24	g	602	CLA	O1D-CGD-O2D-CED
23	G	607	CHL	C2-C3-C5-C6
23	G	608	CHL	C12-C13-C15-C16
23	N	607	CHL	C11-C12-C13-C15
23	Y	308	CHL	C11-C12-C13-C15
23	Y	309	CHL	C12-C13-C15-C16
23	g	607	CHL	C2-C3-C5-C6
23	g	608	CHL	C12-C13-C15-C16
23	n	608	CHL	C12-C13-C15-C16
23	y	309	CHL	C12-C13-C15-C16
23	Au	608	CHL	C12-C13-C15-C16
23	A2	607	CHL	C11-C12-C13-C15
23	BB	308	CHL	C11-C12-C13-C15
23	BJ	607	CHL	C2-C3-C5-C6
23	BJ	608	CHL	C12-C13-C15-C16
23	BQ	608	CHL	C12-C13-C15-C16
23	Ba	309	CHL	C12-C13-C15-C16
24	6	613	CLA	C2-C3-C5-C6
24	B	615	CLA	C11-C10-C8-C7
24	N	603	CLA	C11-C10-C8-C7
24	d	402	CLA	C6-C7-C8-C10
24	n	603	CLA	C11-C10-C8-C7
24	n	611	CLA	C11-C10-C8-C7
24	y	303	CLA	C11-C12-C13-C15
24	y	304	CLA	C2-C3-C5-C6
24	y	313	CLA	C2-C3-C5-C6
24	y	313	CLA	C11-C10-C8-C7
24	C	502	CLA	C11-C10-C8-C7
24	C	502	CLA	C12-C13-C15-C16
24	C	504	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	C	506	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	c	502	CLA	C12-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	507	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
24	9	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	v	602	CLA	C6-C7-C8-C10
24	Au	603	CLA	C11-C10-C8-C7
24	Aw	102	CLA	C2-C3-C5-C6
24	A2	603	CLA	C11-C10-C8-C7
24	A6	602	CLA	C6-C7-C8-C10
24	BB	303	CLA	C6-C7-C8-C10
24	BE	603	CLA	C6-C7-C8-C10
24	BG	402	CLA	C6-C7-C8-C10
24	BQ	603	CLA	C11-C10-C8-C7
24	BQ	611	CLA	C11-C10-C8-C7
24	Ba	303	CLA	C11-C12-C13-C15
24	Ba	313	CLA	C2-C3-C5-C6
24	Ba	313	CLA	C11-C10-C8-C7
24	1	502	CLA	C12-C13-C15-C16
24	1	504	CLA	C12-C13-C15-C16
24	1	506	CLA	C11-C12-C13-C15
24	1	506	CLA	C12-C13-C15-C16
24	1	511	CLA	C11-C12-C13-C15
24	BF	502	CLA	C11-C10-C8-C7
24	BF	502	CLA	C12-C13-C15-C16
24	BF	506	CLA	C2-C3-C5-C6
24	BF	507	CLA	C12-C13-C15-C16
24	BF	508	CLA	C11-C10-C8-C7
38	A	409	PHO	C11-C10-C8-C7
38	a	409	PHO	C11-C10-C8-C7
38	R	408	PHO	C11-C10-C8-C7
38	BD	409	PHO	C11-C10-C8-C7
24	Y	314	CLA	C3-C5-C6-C7
38	BD	409	PHO	C3-C5-C6-C7
24	7	311	CLA	O1A-CGA-O2A-C1
24	c	504	CLA	O1A-CGA-O2A-C1
24	9	603	CLA	O1A-CGA-O2A-C1
24	AA	311	CLA	O1A-CGA-O2A-C1
24	BF	504	CLA	O1A-CGA-O2A-C1
30	C	519	LMG	C30-C31-C32-C33
30	1	519	LMG	C30-C31-C32-C33
30	BF	501	LMG	C34-C35-C36-C37
24	N	613	CLA	C8-C10-C11-C12
24	c	512	CLA	C5-C6-C7-C8
24	v	614	CLA	C5-C6-C7-C8
24	BF	508	CLA	C15-C16-C17-C18
24	BF	511	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	y	318	NEX	C29-C30-C31-C32
26	y	318	NEX	C33-C34-C35-C15
26	r	617	NEX	C33-C34-C35-C15
26	BB	318	NEX	C33-C34-C35-C15
26	BB	320	NEX	C33-C34-C35-C15
26	Ba	318	NEX	C29-C30-C31-C32
28	y	301	XAT	C29-C30-C31-C32
28	BB	301	XAT	C29-C30-C31-C32
28	BB	301	XAT	C33-C34-C35-C15
28	Ba	301	XAT	C29-C30-C31-C32
23	N	607	CHL	C16-C17-C18-C19
24	A2	603	CLA	O1D-CGD-O2D-CED
24	1	511	CLA	O1D-CGD-O2D-CED
30	i	101	LMG	C10-C11-C12-C13
30	BL	101	LMG	C10-C11-C12-C13
34	BD	413	DGD	C1A-C2A-C3A-C4A
23	G	608	CHL	CBA-CGA-O2A-C1
23	Au	608	CHL	CBA-CGA-O2A-C1
24	5	604	CLA	CBA-CGA-O2A-C1
24	N	604	CLA	CBA-CGA-O2A-C1
24	Y	305	CLA	CBA-CGA-O2A-C1
24	Y	313	CLA	CBA-CGA-O2A-C1
24	y	314	CLA	CBA-CGA-O2A-C1
24	A2	604	CLA	CBA-CGA-O2A-C1
24	BB	305	CLA	CBA-CGA-O2A-C1
24	BB	314	CLA	CBA-CGA-O2A-C1
27	r	618	LHG	C24-C23-O8-C6
27	BE	624	LHG	C24-C23-O8-C6
27	BY	201	LHG	C24-C23-O8-C6
34	C	518	DGD	C2A-C1A-O1G-C1G
34	1	518	DGD	C2A-C1A-O1G-C1G
34	a	413	DGD	CCA-CDA-CEA-CFA
34	BD	413	DGD	CCA-CDA-CEA-CFA
23	S	606	CHL	C2A-CAA-CBA-CGA
23	A6	606	CHL	C2A-CAA-CBA-CGA
23	Ba	310	CHL	C2A-CAA-CBA-CGA
24	5	602	CLA	C2A-CAA-CBA-CGA
24	5	610	CLA	C2A-CAA-CBA-CGA
24	6	604	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C2A-CAA-CBA-CGA
24	B	606	CLA	C2A-CAA-CBA-CGA
24	B	608	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	b	609	CLA	C2A-CAA-CBA-CGA
24	0	604	CLA	C2A-CAA-CBA-CGA
24	v	601	CLA	C2A-CAA-CBA-CGA
24	v	606	CLA	C2A-CAA-CBA-CGA
24	v	608	CLA	C2A-CAA-CBA-CGA
24	A2	613	CLA	C2A-CAA-CBA-CGA
24	BE	609	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C5-C6-C7-C8
24	n	602	CLA	C8-C10-C11-C12
24	c	511	CLA	C10-C11-C12-C13
24	r	609	CLA	C15-C16-C17-C18
24	v	607	CLA	C10-C11-C12-C13
24	BQ	602	CLA	C8-C10-C11-C12
24	BF	512	CLA	C5-C6-C7-C8
27	N	618	LHG	C33-C34-C35-C36
30	B	620	LMG	C16-C17-C18-C19
30	B	620	LMG	C33-C34-C35-C36
23	s	607	CHL	C2C-C3C-CAC-CBC
27	1	521	LHG	C27-C28-C29-C30
32	D	406	SQD	C14-C15-C16-C17
23	9	609	CHL	C12-C13-C15-C16
24	0	613	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	C13-C15-C16-C17
24	B	607	CLA	C10-C11-C12-C13
24	v	606	CLA	C13-C15-C16-C17
24	BE	615	CLA	C5-C6-C7-C8
27	BJ	618	LHG	C18-C19-C20-C21
27	1	520	LHG	C33-C34-C35-C36
30	D	405	LMG	C12-C13-C14-C15
30	c	518	LMG	C30-C31-C32-C33
30	BF	519	LMG	C30-C31-C32-C33
32	L	103	SQD	C26-C27-C28-C29
32	L	103	SQD	C31-C32-C33-C34
24	B	615	CLA	C3-C5-C6-C7
24	G	610	CLA	C3-C5-C6-C7
24	Au	610	CLA	C3-C5-C6-C7
24	BB	303	CLA	C3-C5-C6-C7
27	C	521	LHG	C14-C15-C16-C17
30	B	620	LMG	C30-C31-C32-C33
30	C	501	LMG	C34-C35-C36-C37
30	v	620	LMG	C30-C31-C32-C33
32	d	406	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	2	408	SQD	C14-C15-C16-C17
29	8	313	BCR	C6-C7-C8-C9
29	BE	601	BCR	C6-C7-C8-C9
23	6	605	CHL	CBD-CGD-O2D-CED
24	Ba	314	CLA	CBA-CGA-O2A-C1
27	w	201	LHG	C24-C23-O8-C6
27	Ba	319	LHG	C24-C23-O8-C6
23	N	608	CHL	C16-C17-C18-C20
23	Au	607	CHL	C16-C17-C18-C20
23	A2	608	CHL	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
24	BB	311	CLA	C11-C12-C13-C15
32	d	406	SQD	O5-C1-O6-C44
34	a	413	DGD	O6D-C1D-O3G-C3G
34	BD	413	DGD	O6D-C1D-O3G-C3G
24	BU	609	CLA	C15-C16-C17-C18
38	A	409	PHO	C8-C10-C11-C12
24	BJ	602	CLA	O1D-CGD-O2D-CED
24	BV	612	CLA	O1D-CGD-O2D-CED
23	BV	607	CHL	C2C-C3C-CAC-CBC
27	BE	623	LHG	C28-C29-C30-C31
27	BG	404	LHG	C11-C10-C9-C8
30	v	620	LMG	C16-C17-C18-C19
34	C	518	DGD	C3B-C4B-C5B-C6B
34	1	518	DGD	C3B-C4B-C5B-C6B
27	2	405	LHG	C7-C8-C9-C10
27	2	406	LHG	C23-C24-C25-C26
27	b	622	LHG	C8-C7-O7-C5
27	BE	622	LHG	C8-C7-O7-C5
30	B	620	LMG	C11-C10-O7-C8
30	B	624	LMG	C11-C10-O7-C8
30	b	621	LMG	C11-C10-O7-C8
30	v	620	LMG	C11-C10-O7-C8
30	v	623	LMG	C11-C10-O7-C8
30	BE	621	LMG	C11-C10-O7-C8
34	a	413	DGD	C2B-C1B-O2G-C2G
34	BD	413	DGD	C2B-C1B-O2G-C2G
26	AA	319	NEX	C30-C31-C32-C33
29	B	623	BCR	C18-C19-C20-C21
27	C	520	LHG	C15-C16-C17-C18
27	C	520	LHG	C33-C34-C35-C36
27	BJ	618	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	1	520	LHG	C15-C16-C17-C18
30	1	501	LMG	C34-C35-C36-C37
32	l	101	SQD	C26-C27-C28-C29
34	R	401	DGD	CCB-CDB-CEB-CFB
24	y	312	CLA	C5-C6-C7-C8
24	1	510	CLA	C15-C16-C17-C18
23	0	605	CHL	CBD-CGD-O2D-CED
23	Au	607	CHL	CBD-CGD-O2D-CED
27	C	521	LHG	C27-C28-C29-C30
27	0	617	LHG	C32-C33-C34-C35
32	BO	101	SQD	C26-C27-C28-C29
30	c	518	LMG	O9-C10-O7-C8
30	1	519	LMG	O9-C10-O7-C8
30	BF	519	LMG	O9-C10-O7-C8
34	BF	518	DGD	O1B-C1B-O2G-C2G
24	BB	314	CLA	C3-C5-C6-C7
24	1	506	CLA	C3-C5-C6-C7
30	1	519	LMG	C28-C29-C30-C31
27	g	618	LHG	C13-C14-C15-C16
34	R	401	DGD	C6A-C7A-C8A-C9A
24	v	615	CLA	C8-C10-C11-C12
24	Ba	312	CLA	C5-C6-C7-C8
27	5	618	LHG	O7-C5-C6-O8
27	9	618	LHG	O7-C5-C6-O8
32	L	101	SQD	O47-C45-C46-O48
32	l	102	SQD	O47-C45-C46-O48
32	A	413	SQD	O6-C44-C45-O47
32	A	413	SQD	O47-C45-C46-O48
32	a	412	SQD	O47-C45-C46-O48
32	Az	101	SQD	O47-C45-C46-O48
32	BO	102	SQD	O47-C45-C46-O48
32	R	411	SQD	O6-C44-C45-O47
32	R	411	SQD	O47-C45-C46-O48
32	BD	412	SQD	O47-C45-C46-O48
30	BL	101	LMG	O6-C5-C6-O5
32	d	406	SQD	C14-C15-C16-C17
23	Au	609	CHL	C11-C12-C13-C14
24	y	311	CLA	C11-C12-C13-C14
24	BF	507	CLA	C16-C17-C18-C20
30	BE	621	LMG	C32-C33-C34-C35
24	b	615	CLA	C5-C6-C7-C8
24	BJ	611	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	5	607	CHL	C4-C3-C5-C6
23	g	607	CHL	C4-C3-C5-C6
24	Aw	102	CLA	C4-C3-C5-C6
24	BE	616	CLA	C4-C3-C5-C6
31	BG	403	PL9	C45-C44-C46-C47
27	D	404	LHG	C23-C24-C25-C26
23	6	607	CHL	C2-C3-C5-C6
23	0	607	CHL	C2-C3-C5-C6
23	Au	607	CHL	C2-C3-C5-C6
24	I	102	CLA	C2-C3-C5-C6
24	v	614	CLA	C2-C3-C5-C6
24	Ba	304	CLA	C2-C3-C5-C6
27	d	404	LHG	C10-C11-C12-C13
27	2	405	LHG	C28-C29-C30-C31
27	1	521	LHG	C14-C15-C16-C17
34	1	516	DGD	C5A-C6A-C7A-C8A
34	1	518	DGD	C7A-C8A-C9A-CAA
34	BD	413	DGD	C6B-C7B-C8B-C9B
23	n	601	CHL	C11-C12-C13-C14
24	G	603	CLA	C11-C10-C8-C9
24	N	603	CLA	C11-C10-C8-C9
24	Y	303	CLA	C6-C7-C8-C9
24	d	402	CLA	C6-C7-C8-C9
24	g	613	CLA	C14-C13-C15-C16
24	n	603	CLA	C11-C10-C8-C9
24	y	303	CLA	C11-C12-C13-C14
24	c	502	CLA	C11-C10-C8-C9
24	c	503	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C10-C8-C9
24	v	615	CLA	C11-C10-C8-C9
24	Au	603	CLA	C11-C10-C8-C9
24	BG	402	CLA	C6-C7-C8-C9
24	BJ	613	CLA	C14-C13-C15-C16
24	BQ	603	CLA	C11-C10-C8-C9
24	Ba	303	CLA	C11-C12-C13-C14
24	1	513	CLA	C11-C12-C13-C14
24	BF	502	CLA	C11-C10-C8-C9
24	BF	503	CLA	C14-C13-C15-C16
24	BF	506	CLA	C11-C10-C8-C9
24	BF	514	CLA	C11-C12-C13-C14
38	a	408	PHO	C14-C13-C15-C16
24	Ba	313	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	2	404	PL9	C47-C48-C49-C51
27	g	618	LHG	C27-C28-C29-C30
27	BJ	618	LHG	C27-C28-C29-C30
32	BG	406	SQD	C14-C15-C16-C17
34	A	402	DGD	C6A-C7A-C8A-C9A
24	C	506	CLA	C3-C5-C6-C7
23	5	605	CHL	C2A-CAA-CBA-CGA
23	5	607	CHL	C2A-CAA-CBA-CGA
23	9	605	CHL	C2A-CAA-CBA-CGA
23	AB	305	CHL	C2A-CAA-CBA-CGA
24	N	602	CLA	C2A-CAA-CBA-CGA
24	N	613	CLA	C2A-CAA-CBA-CGA
24	Y	314	CLA	C2A-CAA-CBA-CGA
24	g	611	CLA	C2A-CAA-CBA-CGA
24	C	506	CLA	C2A-CAA-CBA-CGA
24	v	612	CLA	C2A-CAA-CBA-CGA
24	Au	604	CLA	C2A-CAA-CBA-CGA
24	A2	602	CLA	C2A-CAA-CBA-CGA
24	BB	314	CLA	C2A-CAA-CBA-CGA
24	BJ	611	CLA	C2A-CAA-CBA-CGA
24	1	506	CLA	C2A-CAA-CBA-CGA
27	6	617	LHG	C32-C33-C34-C35
27	L	102	LHG	C11-C12-C13-C14
32	BO	101	SQD	C31-C32-C33-C34
32	BD	412	SQD	C29-C30-C31-C32
34	A	402	DGD	CCB-CDB-CEB-CFB
34	a	401	DGD	C3B-C4B-C5B-C6B
34	a	413	DGD	C6B-C7B-C8B-C9B
24	N	613	CLA	CBA-CGA-O2A-C1
24	A2	613	CLA	CBA-CGA-O2A-C1
29	h	101	BCR	C7-C8-C9-C34
24	G	610	CLA	C5-C6-C7-C8
24	A6	612	CLA	C5-C6-C7-C8
24	BE	609	CLA	C8-C10-C11-C12
27	b	623	LHG	C32-C33-C34-C35
27	BG	404	LHG	C32-C33-C34-C35
30	Aw	101	LMG	C35-C36-C37-C38
32	D	406	SQD	C27-C28-C29-C30
32	l	101	SQD	C31-C32-C33-C34
34	a	413	DGD	C3B-C4B-C5B-C6B
34	BD	413	DGD	C3B-C4B-C5B-C6B
26	7	319	NEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	9	617	NEX	C31-C32-C33-C34
29	8	313	BCR	C11-C12-C13-C14
29	b	601	BCR	C7-C8-C9-C10
29	b	601	BCR	C11-C12-C13-C14
29	BE	601	BCR	C7-C8-C9-C10
29	BE	601	BCR	C11-C12-C13-C14
23	G	608	CHL	O1A-CGA-O2A-C1
23	Au	608	CHL	O1A-CGA-O2A-C1
24	5	603	CLA	O1A-CGA-O2A-C1
24	S	610	CLA	O1A-CGA-O2A-C1
24	y	305	CLA	O1A-CGA-O2A-C1
24	9	604	CLA	O1A-CGA-O2A-C1
24	A6	610	CLA	O1A-CGA-O2A-C1
23	r	607	CHL	O1D-CGD-O2D-CED
23	5	607	CHL	C1A-C2A-CAA-CBA
23	5	608	CHL	C1A-C2A-CAA-CBA
23	5	609	CHL	C1A-C2A-CAA-CBA
23	6	607	CHL	C1A-C2A-CAA-CBA
23	6	609	CHL	C1A-C2A-CAA-CBA
23	7	310	CHL	C1A-C2A-CAA-CBA
23	8	305	CHL	C1A-C2A-CAA-CBA
23	G	605	CHL	C1A-C2A-CAA-CBA
23	Y	309	CHL	C1A-C2A-CAA-CBA
23	g	609	CHL	C1A-C2A-CAA-CBA
23	y	309	CHL	C1A-C2A-CAA-CBA
23	9	607	CHL	C1A-C2A-CAA-CBA
23	9	608	CHL	C1A-C2A-CAA-CBA
23	9	609	CHL	C1A-C2A-CAA-CBA
23	0	607	CHL	C1A-C2A-CAA-CBA
23	0	609	CHL	C1A-C2A-CAA-CBA
23	AA	307	CHL	C1A-C2A-CAA-CBA
23	AA	310	CHL	C1A-C2A-CAA-CBA
23	Au	605	CHL	C1A-C2A-CAA-CBA
23	A2	609	CHL	C1A-C2A-CAA-CBA
23	BB	309	CHL	C1A-C2A-CAA-CBA
23	BJ	609	CHL	C1A-C2A-CAA-CBA
23	BQ	606	CHL	C1A-C2A-CAA-CBA
23	Ba	309	CHL	C1A-C2A-CAA-CBA
24	5	610	CLA	C1A-C2A-CAA-CBA
24	6	610	CLA	C1A-C2A-CAA-CBA
24	7	312	CLA	C1A-C2A-CAA-CBA
24	8	301	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	8	308	CLA	C1A-C2A-CAA-CBA
24	8	309	CLA	C1A-C2A-CAA-CBA
24	B	609	CLA	C1A-C2A-CAA-CBA
24	B	612	CLA	C1A-C2A-CAA-CBA
24	N	611	CLA	C1A-C2A-CAA-CBA
24	S	602	CLA	C1A-C2A-CAA-CBA
24	S	610	CLA	C1A-C2A-CAA-CBA
24	Y	315	CLA	C1A-C2A-CAA-CBA
24	b	602	CLA	C1A-C2A-CAA-CBA
24	b	610	CLA	C1A-C2A-CAA-CBA
24	b	613	CLA	C1A-C2A-CAA-CBA
24	s	604	CLA	C1A-C2A-CAA-CBA
24	s	610	CLA	C1A-C2A-CAA-CBA
24	y	315	CLA	C1A-C2A-CAA-CBA
24	A	406	CLA	C1A-C2A-CAA-CBA
24	A	407	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	C	511	CLA	C1A-C2A-CAA-CBA
24	a	406	CLA	C1A-C2A-CAA-CBA
24	a	407	CLA	C1A-C2A-CAA-CBA
24	c	502	CLA	C1A-C2A-CAA-CBA
24	r	609	CLA	C1A-C2A-CAA-CBA
24	9	610	CLA	C1A-C2A-CAA-CBA
24	0	610	CLA	C1A-C2A-CAA-CBA
24	AA	312	CLA	C1A-C2A-CAA-CBA
24	AB	301	CLA	C1A-C2A-CAA-CBA
24	AB	309	CLA	C1A-C2A-CAA-CBA
24	v	609	CLA	C1A-C2A-CAA-CBA
24	v	612	CLA	C1A-C2A-CAA-CBA
24	Aw	102	CLA	C1A-C2A-CAA-CBA
24	A2	604	CLA	C1A-C2A-CAA-CBA
24	A2	611	CLA	C1A-C2A-CAA-CBA
24	A6	602	CLA	C1A-C2A-CAA-CBA
24	A6	610	CLA	C1A-C2A-CAA-CBA
24	BB	315	CLA	C1A-C2A-CAA-CBA
24	BE	602	CLA	C1A-C2A-CAA-CBA
24	BE	610	CLA	C1A-C2A-CAA-CBA
24	BE	613	CLA	C1A-C2A-CAA-CBA
24	BV	602	CLA	C1A-C2A-CAA-CBA
24	BV	604	CLA	C1A-C2A-CAA-CBA
24	BV	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	Ba	315	CLA	C1A-C2A-CAA-CBA
24	R	405	CLA	C1A-C2A-CAA-CBA
24	R	406	CLA	C1A-C2A-CAA-CBA
24	1	502	CLA	C1A-C2A-CAA-CBA
24	1	506	CLA	C1A-C2A-CAA-CBA
24	1	511	CLA	C1A-C2A-CAA-CBA
24	BD	406	CLA	C1A-C2A-CAA-CBA
24	BD	407	CLA	C1A-C2A-CAA-CBA
24	BF	502	CLA	C1A-C2A-CAA-CBA
24	BU	609	CLA	C1A-C2A-CAA-CBA
30	i	101	LMG	O6-C5-C6-O5
23	G	609	CHL	C11-C12-C13-C14
23	y	310	CHL	C16-C17-C18-C20
23	Ba	310	CHL	C16-C17-C18-C20
24	Y	311	CLA	C11-C12-C13-C14
24	c	507	CLA	C16-C17-C18-C19
24	BB	311	CLA	C11-C12-C13-C14
24	BF	507	CLA	C16-C17-C18-C19
30	C	519	LMG	O9-C10-O7-C8
34	c	517	DGD	O1B-C1B-O2G-C2G
27	L	102	LHG	C8-C7-O7-C5
27	B	622	LHG	C28-C29-C30-C31
27	2	406	LHG	C10-C11-C12-C13
27	BF	521	LHG	C27-C28-C29-C30
32	BG	406	SQD	C27-C28-C29-C30
34	BD	401	DGD	C3B-C4B-C5B-C6B
26	Ba	318	NEX	C33-C34-C35-C15
28	Y	301	XAT	C29-C30-C31-C32
23	Au	601	CHL	O1D-CGD-O2D-CED
24	6	614	CLA	O1D-CGD-O2D-CED
24	g	611	CLA	C5-C6-C7-C8
24	c	508	CLA	C15-C16-C17-C18
24	A2	610	CLA	C5-C6-C7-C8
24	BU	608	CLA	C5-C6-C7-C8
27	5	618	LHG	C3-O3-P-O6
27	D	404	LHG	C4-O6-P-O3
27	9	618	LHG	C3-O3-P-O6
27	2	406	LHG	C4-O6-P-O3
27	BG	404	LHG	C4-O6-P-O3
23	5	609	CHL	C4C-C3C-CAC-CBC
23	0	607	CHL	C4C-C3C-CAC-CBC
27	BE	624	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	I	101	LMG	C35-C36-C37-C38
32	A1	101	SQD	C26-C27-C28-C29
34	A	402	DGD	C5B-C6B-C7B-C8B
34	R	401	DGD	C5B-C6B-C7B-C8B
24	2	403	CLA	CBD-CGD-O2D-CED
24	Y	303	CLA	C3-C5-C6-C7
24	BF	511	CLA	C3-C5-C6-C7
27	BE	623	LHG	C32-C33-C34-C35
24	Y	314	CLA	O1A-CGA-O2A-C1
23	Y	310	CHL	C13-C15-C16-C17
24	BB	303	CLA	C8-C10-C11-C12
38	a	409	PHO	C8-C10-C11-C12
27	B	621	LHG	O6-C4-C5-C6
27	c	519	LHG	O6-C4-C5-C6
27	v	621	LHG	O6-C4-C5-C6
27	BE	622	LHG	O6-C4-C5-C6
27	BF	520	LHG	O6-C4-C5-C6
23	BU	605	CHL	O1D-CGD-O2D-CED
30	b	621	LMG	C33-C34-C35-C36
34	C	518	DGD	C7A-C8A-C9A-CAA
32	a	412	SQD	C29-C30-C31-C32
30	BG	405	LMG	O6-C5-C6-O5
24	N	610	CLA	C5-C6-C7-C8
24	BF	514	CLA	C13-C15-C16-C17
24	Ba	311	CLA	C11-C12-C13-C14
30	1	519	LMG	C29-C30-C31-C32
34	c	516	DGD	C5A-C6A-C7A-C8A
23	6	607	CHL	C2C-C3C-CAC-CBC
23	y	310	CHL	C4C-C3C-CAC-CBC
27	b	624	LHG	C10-C11-C12-C13
27	d	404	LHG	C32-C33-C34-C35
27	c	520	LHG	C27-C28-C29-C30
27	BF	521	LHG	C13-C14-C15-C16
30	A	412	LMG	C17-C18-C19-C20
30	2	407	LMG	C16-C17-C18-C19
24	c	511	CLA	C3-C5-C6-C7
24	r	608	CLA	C5-C6-C7-C8
24	Au	610	CLA	C5-C6-C7-C8
27	b	623	LHG	C28-C29-C30-C31
27	c	520	LHG	C13-C14-C15-C16
27	Ba	319	LHG	C31-C32-C33-C34
30	D	405	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	s	609	CLA	CBA-CGA-O2A-C1
32	BO	102	SQD	C24-C23-O48-C46
34	A	402	DGD	O1B-C1B-O2G-C2G
23	6	607	CHL	C4-C3-C5-C6
23	0	607	CHL	C4-C3-C5-C6
24	y	304	CLA	C4-C3-C5-C6
24	Ba	304	CLA	C4-C3-C5-C6
32	d	406	SQD	C27-C28-C29-C30
34	C	516	DGD	C5A-C6A-C7A-C8A
34	BF	517	DGD	C5A-C6A-C7A-C8A
23	N	609	CHL	C13-C15-C16-C17
23	A2	609	CHL	C13-C15-C16-C17
38	BD	409	PHO	C8-C10-C11-C12
30	BF	501	LMG	O6-C5-C6-O5
23	G	607	CHL	CBD-CGD-O2D-CED
30	C	519	LMG	C29-C30-C31-C32
30	v	620	LMG	C35-C36-C37-C38
34	H	102	DGD	C1B-C2B-C3B-C4B
34	C	518	DGD	C1A-C2A-C3A-C4A
24	5	604	CLA	O1A-CGA-O2A-C1
24	N	604	CLA	O1A-CGA-O2A-C1
24	A2	604	CLA	O1A-CGA-O2A-C1
24	BB	305	CLA	O1A-CGA-O2A-C1
27	D	404	LHG	C10-C11-C12-C13
27	n	618	LHG	C33-C34-C35-C36
27	BQ	618	LHG	C33-C34-C35-C36
30	B	620	LMG	C35-C36-C37-C38
30	A0	201	LMG	C17-C18-C19-C20
30	BF	519	LMG	C29-C30-C31-C32
24	c	514	CLA	C13-C15-C16-C17
24	B	612	CLA	C2A-CAA-CBA-CGA
24	G	604	CLA	C2A-CAA-CBA-CGA
24	BB	303	CLA	C2A-CAA-CBA-CGA
24	BE	613	CLA	C2A-CAA-CBA-CGA
24	1	508	CLA	C16-C17-C18-C20
24	0	614	CLA	O1D-CGD-O2D-CED
27	G	618	LHG	C4-C5-C6-O8
27	w	201	LHG	C4-C5-C6-O8
27	9	618	LHG	C4-C5-C6-O8
27	Au	618	LHG	C4-C5-C6-O8
27	A0	202	LHG	C4-C5-C6-O8
27	BY	201	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
27	1	521	LHG	C13-C14-C15-C16
30	C	501	LMG	O1-C7-C8-C9
30	C	519	LMG	C7-C8-C9-O8
30	c	501	LMG	O1-C7-C8-C9
30	c	518	LMG	C29-C30-C31-C32
30	BE	621	LMG	C31-C32-C33-C34
30	1	501	LMG	O1-C7-C8-C9
30	1	519	LMG	C7-C8-C9-O8
30	BF	501	LMG	O1-C7-C8-C9
32	L	101	SQD	C44-C45-C46-O48
32	d	406	SQD	C16-C17-C18-C19
32	Az	101	SQD	C44-C45-C46-O48
32	BO	102	SQD	C44-C45-C46-O48
34	A	402	DGD	O1G-C1G-C2G-C3G
34	R	401	DGD	O1G-C1G-C2G-C3G
23	6	601	CHL	C15-C16-C17-C18
23	0	601	CHL	C15-C16-C17-C18
27	2	406	LHG	C24-C25-C26-C27
30	d	405	LMG	C32-C33-C34-C35
30	BG	405	LMG	C32-C33-C34-C35
32	R	411	SQD	C30-C31-C32-C33
34	1	518	DGD	C1A-C2A-C3A-C4A
24	BB	314	CLA	O1A-CGA-O2A-C1
30	C	501	LMG	C8-C7-O1-C1
30	c	501	LMG	C8-C7-O1-C1
30	1	501	LMG	C8-C7-O1-C1
30	BF	501	LMG	C8-C7-O1-C1
34	C	517	DGD	C5D-C6D-O5D-C1E
34	c	517	DGD	C5D-C6D-O5D-C1E
34	1	517	DGD	C5D-C6D-O5D-C1E
34	BF	518	DGD	C5D-C6D-O5D-C1E
32	BD	412	SQD	C9-C10-C11-C12
34	a	413	DGD	C5A-C6A-C7A-C8A
24	S	602	CLA	C10-C11-C12-C13
24	A2	610	CLA	C13-C15-C16-C17
24	BF	507	CLA	C15-C16-C17-C18
34	C	518	DGD	C6B-C7B-C8B-C9B
24	s	612	CLA	O1D-CGD-O2D-CED
30	C	519	LMG	C28-C29-C30-C31
34	Av	102	DGD	C1B-C2B-C3B-C4B
24	Y	305	CLA	O1A-CGA-O2A-C1
24	Y	313	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	AB	307	CHL	C4C-C3C-CAC-CBC
27	Ba	319	LHG	C27-C28-C29-C30
32	a	412	SQD	C9-C10-C11-C12
32	BG	406	SQD	C16-C17-C18-C19
34	BD	413	DGD	C5A-C6A-C7A-C8A
24	C	508	CLA	C16-C17-C18-C20
30	c	501	LMG	O6-C1-O1-C7
30	BF	501	LMG	O6-C1-O1-C7
24	N	602	CLA	C8-C10-C11-C12
30	i	101	LMG	C17-C18-C19-C20
32	A	413	SQD	C30-C31-C32-C33
34	1	518	DGD	C6B-C7B-C8B-C9B
24	d	402	CLA	CBD-CGD-O2D-CED
34	a	401	DGD	O6E-C5E-C6E-O5E
27	y	319	LHG	C27-C28-C29-C30
27	y	319	LHG	C31-C32-C33-C34
32	A	413	SQD	C19-C20-C21-C22
34	a	413	DGD	C5B-C6B-C7B-C8B
24	D	402	CLA	C15-C16-C17-C18
27	BQ	618	LHG	C24-C25-C26-C27
30	BL	101	LMG	C17-C18-C19-C20
32	A1	101	SQD	C35-C36-C37-C38
27	Az	102	LHG	C8-C7-O7-C5
27	C	521	LHG	C13-C14-C15-C16
27	Az	102	LHG	C11-C12-C13-C14
24	5	610	CLA	C5-C6-C7-C8
24	G	602	CLA	C10-C11-C12-C13
24	c	507	CLA	C15-C16-C17-C18
24	2	403	CLA	C15-C16-C17-C18
24	BB	303	CLA	C13-C15-C16-C17
24	1	508	CLA	C13-C15-C16-C17
26	S	616	NEX	C39-C29-C30-C31
26	AA	319	NEX	C20-C13-C14-C15
28	5	619	XAT	C20-C13-C14-C15
28	N	619	XAT	C39-C29-C30-C31
28	n	619	XAT	C20-C13-C14-C15
29	B	623	BCR	C20-C21-C22-C37
30	c	501	LMG	O6-C5-C6-O5
34	BD	401	DGD	O6E-C5E-C6E-O5E
23	BB	308	CHL	C4-C3-C5-C6
24	BB	304	CLA	C4-C3-C5-C6
30	BE	621	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	L	103	SQD	C35-C36-C37-C38
23	g	607	CHL	C16-C17-C18-C19
23	0	609	CHL	C11-C12-C13-C15
23	BJ	607	CHL	C16-C17-C18-C19
23	BQ	609	CHL	C16-C17-C18-C20
23	5	607	CHL	CBA-CGA-O2A-C1
24	b	604	CLA	CBA-CGA-O2A-C1
24	n	604	CLA	CBA-CGA-O2A-C1
24	y	304	CLA	CBA-CGA-O2A-C1
24	BE	604	CLA	CBA-CGA-O2A-C1
24	BQ	604	CLA	CBA-CGA-O2A-C1
27	y	319	LHG	C24-C23-O8-C6
30	A0	201	LMG	C29-C28-O8-C9
32	2	408	SQD	C24-C23-O48-C46
27	W	201	LHG	C24-C25-C26-C27
24	B	609	CLA	C15-C16-C17-C18
24	Y	303	CLA	C8-C10-C11-C12
24	C	507	CLA	C15-C16-C17-C18
24	c	509	CLA	C13-C15-C16-C17
24	Au	602	CLA	C10-C11-C12-C13
24	BE	610	CLA	C15-C16-C17-C18
24	1	507	CLA	C15-C16-C17-C18
27	A0	202	LHG	C24-C25-C26-C27
32	2	408	SQD	C31-C32-C33-C34
32	BG	406	SQD	C31-C32-C33-C34
24	b	613	CLA	C2A-CAA-CBA-CGA
24	d	401	CLA	C2A-CAA-CBA-CGA
24	Au	603	CLA	C2A-CAA-CBA-CGA
24	BE	604	CLA	C2A-CAA-CBA-CGA
24	B	605	CLA	C15-C16-C17-C18
24	N	610	CLA	C13-C15-C16-C17
24	y	312	CLA	C8-C10-C11-C12
24	v	612	CLA	C13-C15-C16-C17
24	BF	509	CLA	C13-C15-C16-C17
23	r	605	CHL	C2-C1-O2A-CGA
24	BE	612	CLA	C2-C1-O2A-CGA
27	2	405	LHG	C11-C10-C9-C8
24	r	604	CLA	CBD-CGD-O2D-CED
30	B	624	LMG	O6-C5-C6-O5
30	d	405	LMG	O6-C5-C6-O5
24	Au	613	CLA	C3-C5-C6-C7
23	7	310	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	B	622	LHG	C11-C10-C9-C8
30	Aw	101	LMG	C37-C38-C39-C40
32	R	411	SQD	C19-C20-C21-C22
34	BD	413	DGD	C5B-C6B-C7B-C8B
23	9	607	CHL	O1D-CGD-O2D-CED
23	BJ	601	CHL	O1D-CGD-O2D-CED
24	b	615	CLA	O1D-CGD-O2D-CED
24	BB	303	CLA	O1D-CGD-O2D-CED
27	D	404	LHG	C29-C30-C31-C32
27	n	618	LHG	C24-C25-C26-C27
27	A2	618	LHG	C25-C26-C27-C28
27	BU	617	LHG	C11-C10-C9-C8
30	B	624	LMG	C39-C40-C41-C42
30	b	621	LMG	C35-C36-C37-C38
32	D	406	SQD	C31-C32-C33-C34
32	d	406	SQD	C31-C32-C33-C34
24	Ba	304	CLA	CBA-CGA-O2A-C1
24	BF	512	CLA	CBA-CGA-O2A-C1
27	Y	319	LHG	C24-C23-O8-C6
27	BU	617	LHG	C24-C23-O8-C6
30	A	412	LMG	C29-C28-O8-C9
32	L	101	SQD	C24-C23-O48-C46
32	l	102	SQD	C24-C23-O48-C46
32	Az	101	SQD	C24-C23-O48-C46
27	BB	319	LHG	O6-C4-C5-O7
23	N	608	CHL	C16-C17-C18-C19
23	n	609	CHL	C16-C17-C18-C20
23	A2	608	CHL	C16-C17-C18-C19
24	BE	603	CLA	C16-C17-C18-C19
34	c	517	DGD	C4B-C5B-C6B-C7B
34	R	401	DGD	C4A-C5A-C6A-C7A
34	BF	518	DGD	C4B-C5B-C6B-C7B
34	A	402	DGD	O6D-C5D-C6D-O5D
34	C	516	DGD	O6D-C5D-C6D-O5D
34	R	401	DGD	O6D-C5D-C6D-O5D
24	b	610	CLA	C15-C16-C17-C18
24	v	608	CLA	C8-C10-C11-C12
23	r	605	CHL	O1D-CGD-O2D-CED
24	N	613	CLA	O1A-CGA-O2A-C1
24	y	314	CLA	O1A-CGA-O2A-C1
24	A2	613	CLA	O1A-CGA-O2A-C1
30	I	101	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
27	BG	404	LHG	C23-C24-C25-C26
23	g	607	CHL	C15-C16-C17-C18
23	BB	310	CHL	C13-C15-C16-C17
24	B	612	CLA	C13-C15-C16-C17
24	S	612	CLA	C5-C6-C7-C8
23	BJ	608	CHL	C3-C5-C6-C7
26	5	617	NEX	C11-C10-C9-C8
26	n	617	NEX	C11-C10-C9-C8
26	AA	319	NEX	C12-C13-C14-C15
29	F	101	BCR	C12-C13-C14-C15
29	c	515	BCR	C20-C21-C22-C23
32	l	102	SQD	C9-C10-C11-C12
34	BD	413	DGD	C7A-C8A-C9A-CAA
30	i	101	LMG	O7-C8-C9-O8
30	C	519	LMG	O7-C8-C9-O8
30	BL	101	LMG	O7-C8-C9-O8
34	C	516	DGD	O2G-C2G-C3G-O3G
34	c	516	DGD	O2G-C2G-C3G-O3G
34	BD	401	DGD	O1G-C1G-C2G-O2G
34	BF	517	DGD	O2G-C2G-C3G-O3G
34	a	413	DGD	C2A-C1A-O1G-C1G
27	Y	319	LHG	C27-C28-C29-C30
30	c	518	LMG	C37-C38-C39-C40
34	C	518	DGD	C5B-C6B-C7B-C8B
34	R	401	DGD	C7B-C8B-C9B-CAB
34	BF	517	DGD	O6D-C5D-C6D-O5D
27	B	621	LHG	O9-C7-O7-C5
27	v	621	LHG	O9-C7-O7-C5
34	C	517	DGD	O1B-C1B-O2G-C2G
34	R	401	DGD	O1B-C1B-O2G-C2G
24	y	303	CLA	C13-C15-C16-C17
24	C	508	CLA	C13-C15-C16-C17
24	A2	602	CLA	C8-C10-C11-C12
24	Ba	314	CLA	O1A-CGA-O2A-C1
32	BO	102	SQD	O10-C23-O48-C46
38	A	409	PHO	CHA-CBD-CGD-O1D
38	A	409	PHO	CHA-CBD-CGD-O2D
38	a	409	PHO	CHA-CBD-CGD-O2D
38	R	408	PHO	CHA-CBD-CGD-O1D
38	R	408	PHO	CHA-CBD-CGD-O2D
38	BD	409	PHO	CHA-CBD-CGD-O1D
38	BD	409	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	AA	310	CHL	C2C-C3C-CAC-CBC
27	5	618	LHG	C27-C28-C29-C30
27	N	618	LHG	C25-C26-C27-C28
27	r	618	LHG	C11-C10-C9-C8
30	A	412	LMG	C37-C38-C39-C40
32	BO	101	SQD	C35-C36-C37-C38
34	A	402	DGD	C4A-C5A-C6A-C7A
34	BF	518	DGD	C6A-C7A-C8A-C9A
27	b	622	LHG	C23-C24-C25-C26
23	Y	308	CHL	C4-C3-C5-C6
23	9	607	CHL	C4-C3-C5-C6
23	AA	308	CHL	C4-C3-C5-C6
24	Y	304	CLA	C4-C3-C5-C6
27	BF	520	LHG	C24-C25-C26-C27
34	A	402	DGD	C7B-C8B-C9B-CAB
34	C	516	DGD	C4D-C5D-C6D-O5D
34	BF	517	DGD	C4D-C5D-C6D-O5D
23	BJ	607	CHL	C15-C16-C17-C18
24	BG	402	CLA	C15-C16-C17-C18
23	G	607	CHL	C12-C13-C15-C16
23	Y	308	CHL	C2-C3-C5-C6
23	g	607	CHL	C12-C13-C15-C16
23	n	601	CHL	C11-C12-C13-C15
23	y	302	CHL	C11-C12-C13-C15
23	BB	308	CHL	C2-C3-C5-C6
23	BB	310	CHL	C12-C13-C15-C16
23	BJ	601	CHL	C11-C12-C13-C15
23	BJ	607	CHL	C12-C13-C15-C16
23	BQ	601	CHL	C11-C12-C13-C15
23	BQ	601	CHL	C12-C13-C15-C16
23	Ba	302	CHL	C11-C12-C13-C15
24	5	602	CLA	C11-C10-C8-C7
24	6	602	CLA	C6-C7-C8-C10
24	6	602	CLA	C11-C10-C8-C7
24	B	602	CLA	C6-C7-C8-C10
24	B	612	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	D	402	CLA	C6-C7-C8-C10
24	G	603	CLA	C11-C10-C8-C7
24	G	610	CLA	C11-C12-C13-C15
24	G	610	CLA	C12-C13-C15-C16
24	N	611	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	Y	303	CLA	C11-C12-C13-C15
24	Y	304	CLA	C2-C3-C5-C6
24	Y	314	CLA	C11-C12-C13-C15
24	b	604	CLA	C12-C13-C15-C16
24	b	617	CLA	C12-C13-C15-C16
24	g	603	CLA	C11-C10-C8-C7
24	g	610	CLA	C11-C10-C8-C7
24	g	610	CLA	C11-C12-C13-C15
24	g	610	CLA	C12-C13-C15-C16
24	g	613	CLA	C6-C7-C8-C10
24	g	613	CLA	C12-C13-C15-C16
24	n	602	CLA	C11-C10-C8-C7
24	s	602	CLA	C11-C10-C8-C7
24	y	314	CLA	C11-C12-C13-C15
24	C	503	CLA	C11-C10-C8-C7
24	C	503	CLA	C12-C13-C15-C16
24	C	504	CLA	C11-C10-C8-C7
24	C	509	CLA	C6-C7-C8-C10
24	C	510	CLA	C12-C13-C15-C16
24	C	513	CLA	C11-C12-C13-C15
24	c	502	CLA	C11-C10-C8-C7
24	c	503	CLA	C12-C13-C15-C16
24	c	510	CLA	C6-C7-C8-C10
24	c	510	CLA	C11-C10-C8-C7
24	c	514	CLA	C11-C12-C13-C15
24	r	609	CLA	C11-C10-C8-C7
24	9	602	CLA	C11-C10-C8-C7
24	0	602	CLA	C6-C7-C8-C10
24	0	602	CLA	C11-C10-C8-C7
24	v	606	CLA	C12-C13-C15-C16
24	v	612	CLA	C11-C10-C8-C7
24	v	615	CLA	C12-C13-C15-C16
24	v	616	CLA	C12-C13-C15-C16
24	2	403	CLA	C6-C7-C8-C10
24	Au	610	CLA	C11-C12-C13-C15
24	Au	610	CLA	C12-C13-C15-C16
24	A2	611	CLA	C11-C10-C8-C7
24	BB	303	CLA	C11-C12-C13-C15
24	BB	304	CLA	C2-C3-C5-C6
24	BB	314	CLA	C11-C12-C13-C15
24	BE	604	CLA	C12-C13-C15-C16
24	BE	617	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	BJ	603	CLA	C11-C10-C8-C7
24	BJ	610	CLA	C11-C10-C8-C7
24	BJ	610	CLA	C12-C13-C15-C16
24	BJ	613	CLA	C6-C7-C8-C10
24	BJ	613	CLA	C12-C13-C15-C16
24	BQ	602	CLA	C11-C10-C8-C7
24	Ba	314	CLA	C11-C12-C13-C15
24	1	502	CLA	C11-C10-C8-C7
24	1	503	CLA	C11-C10-C8-C7
24	1	503	CLA	C12-C13-C15-C16
24	1	504	CLA	C11-C10-C8-C7
24	1	507	CLA	C11-C10-C8-C7
24	1	509	CLA	C6-C7-C8-C10
24	1	513	CLA	C11-C12-C13-C15
24	BF	503	CLA	C12-C13-C15-C16
24	BF	510	CLA	C6-C7-C8-C10
24	BF	510	CLA	C11-C10-C8-C7
24	BF	514	CLA	C11-C12-C13-C15
24	BU	609	CLA	C11-C10-C8-C7
32	BO	101	SQD	O47-C7-C8-C9
24	G	613	CLA	C3-C5-C6-C7
24	s	612	CLA	C3-C5-C6-C7
23	g	601	CHL	C11-C12-C13-C14
23	n	607	CHL	C11-C12-C13-C14
23	y	308	CHL	C11-C12-C13-C14
23	Au	607	CHL	C11-C12-C13-C14
23	BJ	601	CHL	C11-C12-C13-C14
23	BQ	601	CHL	C11-C12-C13-C14
23	BQ	601	CHL	C14-C13-C15-C16
23	BQ	607	CHL	C11-C12-C13-C14
23	Ba	308	CHL	C11-C12-C13-C14
24	6	602	CLA	C6-C7-C8-C9
24	B	615	CLA	C11-C12-C13-C14
24	B	616	CLA	C14-C13-C15-C16
24	D	402	CLA	C6-C7-C8-C9
24	G	610	CLA	C14-C13-C15-C16
24	G	613	CLA	C14-C13-C15-C16
24	N	610	CLA	C11-C12-C13-C14
24	Y	303	CLA	C11-C12-C13-C14
24	b	605	CLA	C14-C13-C15-C16
24	b	616	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	g	603	CLA	C11-C10-C8-C9
24	g	610	CLA	C11-C12-C13-C14
24	g	610	CLA	C14-C13-C15-C16
24	n	602	CLA	C11-C12-C13-C14
24	n	610	CLA	C11-C12-C13-C14
24	n	613	CLA	C6-C7-C8-C9
24	C	502	CLA	C11-C10-C8-C9
24	C	503	CLA	C11-C10-C8-C9
24	C	503	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C12-C13-C14
24	c	507	CLA	C11-C12-C13-C14
24	c	514	CLA	C11-C12-C13-C14
24	r	609	CLA	C11-C10-C8-C9
24	9	602	CLA	C11-C12-C13-C14
24	0	602	CLA	C6-C7-C8-C9
24	v	615	CLA	C14-C13-C15-C16
24	v	616	CLA	C14-C13-C15-C16
24	2	403	CLA	C6-C7-C8-C9
24	Au	610	CLA	C14-C13-C15-C16
24	Au	613	CLA	C14-C13-C15-C16
24	A2	602	CLA	C6-C7-C8-C9
24	A2	610	CLA	C11-C12-C13-C14
24	BB	303	CLA	C11-C12-C13-C14
24	BE	616	CLA	C11-C12-C13-C14
24	BE	616	CLA	C14-C13-C15-C16
24	BE	617	CLA	C14-C13-C15-C16
24	BJ	603	CLA	C11-C10-C8-C9
24	BJ	610	CLA	C11-C12-C13-C14
24	BJ	610	CLA	C14-C13-C15-C16
24	BQ	610	CLA	C11-C12-C13-C14
24	BQ	613	CLA	C6-C7-C8-C9
24	Ba	314	CLA	C14-C13-C15-C16
24	1	502	CLA	C11-C10-C8-C9
24	1	503	CLA	C11-C10-C8-C9
24	1	503	CLA	C14-C13-C15-C16
24	BF	507	CLA	C11-C12-C13-C14
24	BU	609	CLA	C11-C10-C8-C9
38	A	408	PHO	C14-C13-C15-C16
24	0	602	CLA	CBD-CGD-O2D-CED
30	BF	501	LMG	C28-C29-C30-C31
27	B	622	LHG	C30-C31-C32-C33
27	BJ	618	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	BF	520	LHG	C33-C34-C35-C36
30	i	101	LMG	C37-C38-C39-C40
30	A0	201	LMG	C37-C38-C39-C40
32	L	101	SQD	C29-C30-C31-C32
32	Az	101	SQD	C29-C30-C31-C32
34	c	517	DGD	C6A-C7A-C8A-C9A
34	R	401	DGD	C3B-C4B-C5B-C6B
24	a	406	CLA	CBA-CGA-O2A-C1
24	BB	313	CLA	CBA-CGA-O2A-C1
24	Ba	313	CLA	CBA-CGA-O2A-C1
34	BD	413	DGD	C2A-C1A-O1G-C1G
24	v	604	CLA	C8-C10-C11-C12
24	BQ	610	CLA	C13-C15-C16-C17
24	Ba	312	CLA	C8-C10-C11-C12
23	8	307	CHL	C2A-CAA-CBA-CGA
23	y	306	CHL	C2A-CAA-CBA-CGA
23	9	606	CHL	C2A-CAA-CBA-CGA
23	Ba	306	CHL	C2A-CAA-CBA-CGA
24	b	604	CLA	C2A-CAA-CBA-CGA
24	BF	508	CLA	C2A-CAA-CBA-CGA
32	BO	102	SQD	C9-C10-C11-C12
23	g	601	CHL	O1D-CGD-O2D-CED
34	c	516	DGD	C4D-C5D-C6D-O5D
25	7	316	LUT	C7-C8-C9-C19
25	Y	316	LUT	C7-C8-C9-C19
25	BB	316	LUT	C7-C8-C9-C19
29	BK	101	BCR	C7-C8-C9-C34
23	6	609	CHL	C11-C12-C13-C15
23	Au	608	CHL	C16-C17-C18-C20
24	1	508	CLA	C16-C17-C18-C19
27	y	319	LHG	C32-C33-C34-C35
27	c	519	LHG	C24-C25-C26-C27
30	BE	621	LMG	C35-C36-C37-C38
30	BF	519	LMG	C37-C38-C39-C40
32	l	101	SQD	C35-C36-C37-C38
34	a	413	DGD	C7A-C8A-C9A-CAA
27	n	618	LHG	O1-C1-C2-C3
27	BE	623	LHG	O1-C1-C2-C3
26	BQ	617	NEX	C31-C32-C33-C34
29	8	313	BCR	C17-C18-C19-C20
29	f	101	BCR	C21-C22-C23-C24
29	h	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	BK	101	BCR	C7-C8-C9-C10
23	9	609	CHL	C4C-C3C-CAC-CBC
27	0	617	LHG	C28-C29-C30-C31
27	BG	404	LHG	C27-C28-C29-C30
30	d	405	LMG	C14-C15-C16-C17
30	v	623	LMG	C39-C40-C41-C42
30	2	407	LMG	C31-C32-C33-C34
32	A	413	SQD	C11-C10-C9-C8
34	C	517	DGD	C4B-C5B-C6B-C7B
34	c	516	DGD	O6D-C5D-C6D-O5D
24	N	602	CLA	C10-C11-C12-C13
24	d	402	CLA	C15-C16-C17-C18
24	n	610	CLA	C13-C15-C16-C17
27	g	618	LHG	C12-C13-C14-C15
30	BL	101	LMG	C19-C20-C21-C22
30	BL	101	LMG	C37-C38-C39-C40
24	s	610	CLA	CBA-CGA-O2A-C1
24	y	313	CLA	CBA-CGA-O2A-C1
24	BV	609	CLA	CBA-CGA-O2A-C1
24	BU	604	CLA	CBA-CGA-O2A-C1
27	BB	319	LHG	C24-C23-O8-C6
32	BG	406	SQD	C24-C23-O48-C46
23	S	607	CHL	C2C-C3C-CAC-CBC
27	d	404	LHG	C27-C28-C29-C30
30	i	101	LMG	C19-C20-C21-C22
34	A	402	DGD	C3B-C4B-C5B-C6B
30	c	501	LMG	C28-C29-C30-C31
24	B	605	CLA	C13-C15-C16-C17
24	B	608	CLA	C8-C10-C11-C12
24	Y	303	CLA	C13-C15-C16-C17
24	v	604	CLA	C5-C6-C7-C8
24	Ba	303	CLA	C13-C15-C16-C17
32	l	101	SQD	O47-C7-C8-C9
23	g	608	CHL	C3-C5-C6-C7
30	v	623	LMG	O6-C5-C6-O5
29	AB	313	BCR	C6-C7-C8-C9
29	v	622	BCR	C22-C23-C24-C25
29	4	101	BCR	C6-C7-C8-C9
27	c	519	LHG	C33-C34-C35-C36
30	BG	405	LMG	C14-C15-C16-C17
23	y	308	CHL	C4B-C3B-CAB-CBB
24	5	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	5	611	CLA	C4B-C3B-CAB-CBB
24	6	613	CLA	C4B-C3B-CAB-CBB
24	8	303	CLA	C4B-C3B-CAB-CBB
24	B	615	CLA	C4B-C3B-CAB-CBB
24	G	610	CLA	C4B-C3B-CAB-CBB
24	G	611	CLA	C4B-C3B-CAB-CBB
24	S	611	CLA	C4B-C3B-CAB-CBB
24	b	616	CLA	C4B-C3B-CAB-CBB
24	n	613	CLA	C4B-C3B-CAB-CBB
24	s	608	CLA	C4B-C3B-CAB-CBB
24	s	613	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
24	r	608	CLA	C4B-C3B-CAB-CBB
24	9	604	CLA	C4B-C3B-CAB-CBB
24	0	612	CLA	C4B-C3B-CAB-CBB
24	0	613	CLA	C4B-C3B-CAB-CBB
24	AB	303	CLA	C4B-C3B-CAB-CBB
24	v	615	CLA	C4B-C3B-CAB-CBB
24	Au	611	CLA	C4B-C3B-CAB-CBB
24	A2	603	CLA	C4B-C3B-CAB-CBB
24	A6	611	CLA	C4B-C3B-CAB-CBB
24	BE	616	CLA	C4B-C3B-CAB-CBB
24	BQ	613	CLA	C4B-C3B-CAB-CBB
24	BV	613	CLA	C4B-C3B-CAB-CBB
24	1	511	CLA	C4B-C3B-CAB-CBB
24	BD	405	CLA	C4B-C3B-CAB-CBB
30	B	624	LMG	C4-C5-C6-O5
32	BG	406	SQD	O5-C1-O6-C44
24	B	604	CLA	C5-C6-C7-C8
24	B	604	CLA	C8-C10-C11-C12
24	n	603	CLA	C10-C11-C12-C13
24	A2	602	CLA	C10-C11-C12-C13
27	b	622	LHG	O6-C4-C5-C6
27	C	520	LHG	O6-C4-C5-C6
27	1	520	LHG	O6-C4-C5-C6
24	Y	311	CLA	C3-C5-C6-C7
24	BV	602	CLA	C3-C5-C6-C7
24	BE	615	CLA	O1D-CGD-O2D-CED
24	R	406	CLA	O1D-CGD-O2D-CED
27	Ba	319	LHG	C32-C33-C34-C35
34	1	517	DGD	C4B-C5B-C6B-C7B
27	d	404	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	BB	319	LHG	C23-C24-C25-C26
27	9	618	LHG	C10-C11-C12-C13
27	2	405	LHG	C30-C31-C32-C33
27	BE	623	LHG	C11-C10-C9-C8
24	C	503	CLA	CBA-CGA-O2A-C1
24	BV	610	CLA	CBA-CGA-O2A-C1
24	6	610	CLA	C8-C10-C11-C12
24	g	602	CLA	C10-C11-C12-C13
24	0	610	CLA	C8-C10-C11-C12
24	Au	603	CLA	C5-C6-C7-C8
24	A2	611	CLA	C10-C11-C12-C13
24	BD	405	CLA	C13-C15-C16-C17
23	G	601	CHL	O1D-CGD-O2D-CED
30	c	518	LMG	C19-C20-C21-C22
23	y	308	CHL	C4-C3-C5-C6
23	Ba	308	CHL	C4-C3-C5-C6
24	Y	314	CLA	C4-C3-C5-C6
24	b	608	CLA	C4-C3-C5-C6
24	BV	609	CLA	C4-C3-C5-C6
23	AA	308	CHL	C2-C3-C5-C6
34	BK	102	DGD	C1A-C2A-C3A-C4A
24	N	611	CLA	C10-C11-C12-C13
24	a	405	CLA	C13-C15-C16-C17
27	BU	617	LHG	O2-C2-C3-O3
27	BY	201	LHG	C24-C25-C26-C27
30	A0	201	LMG	C19-C20-C21-C22
34	1	517	DGD	C6A-C7A-C8A-C9A
24	BG	401	CLA	C3-C5-C6-C7
34	R	401	DGD	C4D-C5D-C6D-O5D
34	1	516	DGD	C4D-C5D-C6D-O5D
23	G	608	CHL	C16-C17-C18-C20
24	C	508	CLA	C16-C17-C18-C19
24	r	602	CLA	C11-C12-C13-C15
24	BF	509	CLA	C16-C17-C18-C20
24	BU	602	CLA	C11-C12-C13-C15
34	C	517	DGD	C6A-C7A-C8A-C9A
24	G	603	CLA	C5-C6-C7-C8
24	B	602	CLA	CBA-CGA-O2A-C1
24	c	503	CLA	CBA-CGA-O2A-C1
34	1	516	DGD	O6D-C5D-C6D-O5D
27	BE	622	LHG	C23-C24-C25-C26
27	b	623	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	b	604	CLA	O1A-CGA-O2A-C1
24	y	304	CLA	O1A-CGA-O2A-C1
24	BE	604	CLA	O1A-CGA-O2A-C1
32	2	408	SQD	O10-C23-O48-C46
23	6	601	CHL	C3A-C2A-CAA-CBA
23	7	302	CHL	C3A-C2A-CAA-CBA
23	Y	308	CHL	C3A-C2A-CAA-CBA
23	g	601	CHL	C3A-C2A-CAA-CBA
23	g	605	CHL	C3A-C2A-CAA-CBA
23	g	607	CHL	C3A-C2A-CAA-CBA
23	n	601	CHL	C3A-C2A-CAA-CBA
23	AA	302	CHL	C3A-C2A-CAA-CBA
23	AB	305	CHL	C3A-C2A-CAA-CBA
23	BJ	601	CHL	C3A-C2A-CAA-CBA
23	BJ	605	CHL	C3A-C2A-CAA-CBA
23	BJ	607	CHL	C3A-C2A-CAA-CBA
23	BQ	601	CHL	C3A-C2A-CAA-CBA
24	B	606	CLA	C3A-C2A-CAA-CBA
24	B	607	CLA	C3A-C2A-CAA-CBA
24	I	102	CLA	C3A-C2A-CAA-CBA
24	N	604	CLA	C3A-C2A-CAA-CBA
24	b	602	CLA	C3A-C2A-CAA-CBA
24	b	609	CLA	C3A-C2A-CAA-CBA
24	c	503	CLA	C3A-C2A-CAA-CBA
24	v	606	CLA	C3A-C2A-CAA-CBA
24	v	607	CLA	C3A-C2A-CAA-CBA
24	Aw	102	CLA	C3A-C2A-CAA-CBA
24	A2	604	CLA	C3A-C2A-CAA-CBA
24	A6	604	CLA	C3A-C2A-CAA-CBA
24	BE	602	CLA	C3A-C2A-CAA-CBA
24	BE	609	CLA	C3A-C2A-CAA-CBA
24	BF	503	CLA	C3A-C2A-CAA-CBA
24	b	605	CLA	C13-C15-C16-C17
24	9	610	CLA	C5-C6-C7-C8
23	8	307	CHL	C4C-C3C-CAC-CBC
30	A	412	LMG	C19-C20-C21-C22
26	Ba	318	NEX	C9-C10-C11-C12
28	Y	301	XAT	C13-C14-C15-C35
28	g	619	XAT	C13-C14-C15-C35
28	BJ	619	XAT	C13-C14-C15-C35
28	BQ	619	XAT	C33-C34-C35-C15
34	A	402	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
27	5	618	LHG	C10-C11-C12-C13
27	9	618	LHG	C27-C28-C29-C30
27	Au	618	LHG	C24-C25-C26-C27
27	BU	617	LHG	C28-C29-C30-C31
34	1	518	DGD	C5B-C6B-C7B-C8B
24	A	407	CLA	O1D-CGD-O2D-CED
24	N	613	CLA	C3-C5-C6-C7
24	BV	612	CLA	C3-C5-C6-C7
27	r	618	LHG	C28-C29-C30-C31
30	1	519	LMG	C36-C37-C38-C39
32	D	406	SQD	C16-C17-C18-C19
23	9	607	CHL	CBA-CGA-O2A-C1
24	r	604	CLA	CBA-CGA-O2A-C1
24	Au	611	CLA	CBA-CGA-O2A-C1
24	BD	406	CLA	CBA-CGA-O2A-C1
32	d	406	SQD	C24-C23-O48-C46
27	0	617	LHG	C30-C31-C32-C33
32	A	413	SQD	C9-C10-C11-C12
23	A2	601	CHL	C3-C5-C6-C7
24	v	609	CLA	C15-C16-C17-C18
24	BE	605	CLA	C13-C15-C16-C17
24	BQ	603	CLA	C10-C11-C12-C13
27	5	618	LHG	C4-C5-C6-O8
27	W	201	LHG	C4-C5-C6-O8
27	c	520	LHG	C4-C5-C6-O8
27	BF	521	LHG	C4-C5-C6-O8
30	i	101	LMG	C7-C8-C9-O8
30	A	412	LMG	C7-C8-C9-O8
30	c	518	LMG	C7-C8-C9-O8
30	BL	101	LMG	C7-C8-C9-O8
30	BF	519	LMG	C7-C8-C9-O8
32	l	102	SQD	C44-C45-C46-O48
32	A	413	SQD	O6-C44-C45-C46
32	A	413	SQD	C44-C45-C46-O48
32	a	412	SQD	O6-C44-C45-C46
32	a	412	SQD	C44-C45-C46-O48
32	R	411	SQD	C44-C45-C46-O48
32	BD	412	SQD	O6-C44-C45-C46
32	BD	412	SQD	C44-C45-C46-O48
34	A	402	DGD	C1G-C2G-C3G-O3G
34	a	401	DGD	O1G-C1G-C2G-C3G
34	c	516	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
34	R	401	DGD	C1G-C2G-C3G-O3G
34	BD	401	DGD	O1G-C1G-C2G-C3G
34	BF	517	DGD	C1G-C2G-C3G-O3G
34	1	517	DGD	O1B-C1B-O2G-C2G
30	c	501	LMG	C15-C16-C17-C18
30	BF	519	LMG	C19-C20-C21-C22
32	R	411	SQD	C11-C10-C9-C8
27	v	621	LHG	C23-C24-C25-C26
23	5	607	CHL	O1A-CGA-O2A-C1
24	s	609	CLA	O1A-CGA-O2A-C1
24	BF	512	CLA	O1A-CGA-O2A-C1
32	l	102	SQD	O10-C23-O48-C46
27	w	201	LHG	C24-C25-C26-C27
27	BB	319	LHG	C27-C28-C29-C30
30	b	621	LMG	C16-C17-C18-C19
32	L	101	SQD	C25-C26-C27-C28
27	6	617	LHG	C28-C29-C30-C31
27	g	618	LHG	C30-C31-C32-C33
32	Az	101	SQD	C25-C26-C27-C28
24	Ba	304	CLA	O1A-CGA-O2A-C1
24	N	611	CLA	C4-C3-C5-C6
24	BB	314	CLA	C4-C3-C5-C6
31	d	403	PL9	C45-C44-C46-C47
31	2	404	PL9	C20-C19-C21-C22
23	N	607	CHL	C16-C17-C18-C20
23	y	302	CHL	C16-C17-C18-C20
23	Ba	308	CHL	C16-C17-C18-C20
24	c	509	CLA	C16-C17-C18-C20
23	y	302	CHL	C2-C3-C5-C6
32	2	408	SQD	C16-C17-C18-C19
30	BE	621	LMG	C16-C17-C18-C19
30	BF	501	LMG	C15-C16-C17-C18
34	H	102	DGD	C6A-C7A-C8A-C9A
24	n	603	CLA	C5-C6-C7-C8
24	v	605	CLA	C15-C16-C17-C18
30	v	623	LMG	C4-C5-C6-O5
23	6	608	CHL	C3C-C2C-CMC-OMC
23	N	605	CHL	C3C-C2C-CMC-OMC
23	9	609	CHL	C3C-C2C-CMC-OMC
23	AA	308	CHL	C3C-C2C-CMC-OMC
23	Au	601	CHL	C3C-C2C-CMC-OMC
23	A2	605	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
23	BU	605	CHL	C3C-C2C-CMC-OMC
23	BU	613	CHL	C3C-C2C-CMC-OMC
27	B	621	LHG	C23-C24-C25-C26
27	Y	319	LHG	C23-C24-C25-C26
27	r	618	LHG	C23-C24-C25-C26
27	BG	404	LHG	C7-C8-C9-C10
27	BU	617	LHG	C23-C24-C25-C26
24	BQ	604	CLA	O1A-CGA-O2A-C1
30	C	519	LMG	C36-C37-C38-C39
32	l	101	SQD	C33-C34-C35-C36
32	R	411	SQD	C9-C10-C11-C12
24	A	406	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	C2A-CAA-CBA-CGA
27	b	624	LHG	O1-C1-C2-O2
24	BE	605	CLA	C5-C6-C7-C8
27	n	618	LHG	C13-C14-C15-C16
27	2	406	LHG	C30-C31-C32-C33
27	6	617	LHG	O6-C4-C5-O7
27	B	621	LHG	O6-C4-C5-O7
27	Y	319	LHG	O6-C4-C5-O7
27	y	319	LHG	O6-C4-C5-O7
27	0	617	LHG	O6-C4-C5-O7
27	Ba	319	LHG	O6-C4-C5-O7
24	v	602	CLA	CBA-CGA-O2A-C1
24	1	503	CLA	CBA-CGA-O2A-C1
30	D	405	LMG	C31-C32-C33-C34
30	A0	201	LMG	C31-C32-C33-C34
32	BO	102	SQD	C25-C26-C27-C28
24	n	604	CLA	O1A-CGA-O2A-C1
32	L	101	SQD	O10-C23-O48-C46
32	Az	101	SQD	O10-C23-O48-C46
27	d	404	LHG	C23-C24-C25-C26
23	G	601	CHL	C16-C17-C18-C20
23	N	609	CHL	C16-C17-C18-C19
23	n	607	CHL	C16-C17-C18-C20
23	n	609	CHL	C16-C17-C18-C19
23	y	308	CHL	C16-C17-C18-C20
23	A2	609	CHL	C16-C17-C18-C19
23	BQ	609	CHL	C16-C17-C18-C19
23	Ba	302	CHL	C16-C17-C18-C20
24	v	607	CLA	C16-C17-C18-C20
24	BV	612	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	6	610	CLA	C5-C6-C7-C8
32	BO	101	SQD	C32-C33-C34-C35
24	s	613	CLA	C2B-C3B-CAB-CBB
24	r	608	CLA	C2B-C3B-CAB-CBB
24	0	612	CLA	C2B-C3B-CAB-CBB
24	0	613	CLA	C2B-C3B-CAB-CBB
24	v	615	CLA	C2B-C3B-CAB-CBB
24	A2	603	CLA	C2B-C3B-CAB-CBB
24	A6	611	CLA	C2B-C3B-CAB-CBB
24	BV	613	CLA	C2B-C3B-CAB-CBB
24	1	511	CLA	C2B-C3B-CAB-CBB
24	BD	405	CLA	C2B-C3B-CAB-CBB
27	r	618	LHG	O2-C2-C3-O3
24	c	505	CLA	C2C-C3C-CAC-CBC
30	d	405	LMG	C34-C35-C36-C37
32	l	102	SQD	C25-C26-C27-C28
24	b	605	CLA	C5-C6-C7-C8
24	BJ	602	CLA	C10-C11-C12-C13
24	BQ	603	CLA	C5-C6-C7-C8
24	a	406	CLA	O1A-CGA-O2A-C1
24	BB	313	CLA	O1A-CGA-O2A-C1
27	BQ	618	LHG	C13-C14-C15-C16
32	BO	101	SQD	C33-C34-C35-C36
24	BJ	614	CLA	O2A-C1-C2-C3
27	G	618	LHG	C24-C25-C26-C27
27	BG	404	LHG	C24-C25-C26-C27
27	G	618	LHG	O7-C5-C6-O8
27	W	201	LHG	O7-C5-C6-O8
27	w	201	LHG	O7-C5-C6-O8
27	Au	618	LHG	O7-C5-C6-O8
27	A0	202	LHG	O7-C5-C6-O8
27	BY	201	LHG	O7-C5-C6-O8
30	C	501	LMG	O1-C7-C8-O7
30	c	501	LMG	O1-C7-C8-O7
30	1	501	LMG	O1-C7-C8-O7
30	1	519	LMG	O7-C8-C9-O8
30	BF	501	LMG	O1-C7-C8-O7
34	a	401	DGD	O1G-C1G-C2G-O2G
30	b	621	LMG	C29-C28-O8-C9
27	5	618	LHG	C12-C13-C14-C15
30	C	519	LMG	C37-C38-C39-C40
34	Av	102	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
23	6	609	CHL	C11-C12-C13-C14
23	g	601	CHL	C16-C17-C18-C20
23	A2	607	CHL	C16-C17-C18-C20
30	2	407	LMG	C11-C12-C13-C14
32	l	101	SQD	C32-C33-C34-C35
34	c	516	DGD	O6D-C1D-O3G-C3G
34	BF	517	DGD	O6D-C1D-O3G-C3G
24	D	402	CLA	CBD-CGD-O2D-CED
30	D	405	LMG	C11-C12-C13-C14
30	1	519	LMG	C37-C38-C39-C40
27	b	622	LHG	O9-C7-O7-C5
27	BE	622	LHG	O9-C7-O7-C5
23	BU	605	CHL	C2-C1-O2A-CGA
24	7	303	CLA	C2-C1-O2A-CGA
24	7	311	CLA	C2-C1-O2A-CGA
24	B	611	CLA	C2-C1-O2A-CGA
24	D	401	CLA	C2-C1-O2A-CGA
24	b	612	CLA	C2-C1-O2A-CGA
24	AA	311	CLA	C2-C1-O2A-CGA
24	v	611	CLA	C2-C1-O2A-CGA
24	2	402	CLA	C2-C1-O2A-CGA
31	d	403	PL9	C47-C48-C49-C51
34	R	401	DGD	C4E-C5E-C6E-O5E
23	y	308	CHL	C2-C3-C5-C6
23	Ba	308	CHL	C2-C3-C5-C6
27	BJ	618	LHG	C30-C31-C32-C33
30	C	501	LMG	C35-C36-C37-C38
30	BG	405	LMG	C34-C35-C36-C37
34	BK	102	DGD	C6B-C7B-C8B-C9B
27	Az	102	LHG	O10-C23-O8-C6
24	v	613	CLA	C5-C6-C7-C8
23	G	607	CHL	C11-C12-C13-C14
23	g	607	CHL	C11-C12-C13-C14
23	BJ	607	CHL	C11-C12-C13-C14
24	5	602	CLA	C6-C7-C8-C9
24	5	602	CLA	C11-C12-C13-C14
24	B	605	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	N	602	CLA	C6-C7-C8-C9
24	N	602	CLA	C11-C10-C8-C9
24	N	613	CLA	C6-C7-C8-C9
24	Y	312	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	616	CLA	C11-C12-C13-C14
24	b	617	CLA	C11-C10-C8-C9
24	y	314	CLA	C14-C13-C15-C16
24	c	503	CLA	C11-C10-C8-C9
24	c	513	CLA	C6-C7-C8-C9
24	9	602	CLA	C6-C7-C8-C9
24	v	605	CLA	C14-C13-C15-C16
24	v	615	CLA	C11-C12-C13-C14
24	A2	613	CLA	C6-C7-C8-C9
24	BB	312	CLA	C6-C7-C8-C9
24	BE	605	CLA	C14-C13-C15-C16
24	BE	617	CLA	C11-C10-C8-C9
24	BQ	602	CLA	C11-C12-C13-C14
24	1	510	CLA	C14-C13-C15-C16
24	BF	503	CLA	C11-C10-C8-C9
24	BF	513	CLA	C6-C7-C8-C9
38	BD	408	PHO	C14-C13-C15-C16
27	Au	618	LHG	C13-C14-C15-C16
30	1	501	LMG	C35-C36-C37-C38
24	v	605	CLA	C10-C11-C12-C13
24	A6	602	CLA	C10-C11-C12-C13
24	BQ	613	CLA	C8-C10-C11-C12
27	D	404	LHG	C2-C3-O3-P
27	2	406	LHG	C2-C3-O3-P
27	L	102	LHG	O10-C23-O8-C6
27	c	519	LHG	C13-C14-C15-C16
27	A0	202	LHG	C30-C31-C32-C33
27	BB	319	LHG	C30-C31-C32-C33
27	BG	404	LHG	C34-C35-C36-C37
30	I	101	LMG	C31-C32-C33-C34
30	i	101	LMG	C31-C32-C33-C34
30	Aw	101	LMG	C31-C32-C33-C34
30	1	519	LMG	C18-C19-C20-C21
32	a	412	SQD	C19-C20-C21-C22
34	BF	518	DGD	C8B-C9B-CAB-CBB
23	5	601	CHL	C2A-CAA-CBA-CGA
24	8	301	CLA	C2A-CAA-CBA-CGA
24	G	603	CLA	C2A-CAA-CBA-CGA
24	AB	301	CLA	C2A-CAA-CBA-CGA
24	BF	503	CLA	C2A-CAA-CBA-CGA
23	Y	308	CHL	C16-C17-C18-C20
23	y	302	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	y	310	CHL	C16-C17-C18-C19
23	0	609	CHL	C11-C12-C13-C14
23	BB	310	CHL	C16-C17-C18-C19
23	BJ	601	CHL	C16-C17-C18-C20
23	BJ	608	CHL	C16-C17-C18-C20
23	BQ	607	CHL	C16-C17-C18-C20
23	Ba	310	CHL	C16-C17-C18-C19
24	BE	602	CLA	C16-C17-C18-C20
25	6	616	LUT	C1-C6-C7-C8
25	7	317	LUT	C1-C6-C7-C8
25	8	311	LUT	C1-C6-C7-C8
25	Y	317	LUT	C1-C6-C7-C8
25	g	616	LUT	C1-C6-C7-C8
25	n	616	LUT	C1-C6-C7-C8
25	s	615	LUT	C1-C6-C7-C8
25	9	615	LUT	C1-C6-C7-C8
25	9	616	LUT	C1-C6-C7-C8
25	0	616	LUT	C1-C6-C7-C8
25	AA	317	LUT	C1-C6-C7-C8
25	A2	616	LUT	C1-C6-C7-C8
25	BB	317	LUT	C1-C6-C7-C8
25	BJ	616	LUT	C1-C6-C7-C8
25	BQ	616	LUT	C1-C6-C7-C8
25	BV	615	LUT	C1-C6-C7-C8
29	8	313	BCR	C23-C24-C25-C26
29	B	618	BCR	C1-C6-C7-C8
29	B	618	BCR	C5-C6-C7-C8
29	B	618	BCR	C23-C24-C25-C26
29	B	618	BCR	C23-C24-C25-C30
29	B	619	BCR	C23-C24-C25-C30
29	B	623	BCR	C1-C6-C7-C8
29	B	623	BCR	C5-C6-C7-C8
29	b	619	BCR	C5-C6-C7-C8
29	b	619	BCR	C23-C24-C25-C26
29	A	411	BCR	C1-C6-C7-C8
29	A	411	BCR	C5-C6-C7-C8
29	A	411	BCR	C23-C24-C25-C26
29	A	411	BCR	C23-C24-C25-C30
29	C	515	BCR	C23-C24-C25-C26
29	C	515	BCR	C23-C24-C25-C30
29	a	411	BCR	C1-C6-C7-C8
29	c	515	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	c	515	BCR	C23-C24-C25-C26
29	c	515	BCR	C23-C24-C25-C30
29	AB	313	BCR	C23-C24-C25-C26
29	AB	313	BCR	C23-C24-C25-C30
29	v	618	BCR	C1-C6-C7-C8
29	v	618	BCR	C5-C6-C7-C8
29	v	618	BCR	C23-C24-C25-C26
29	v	618	BCR	C23-C24-C25-C30
29	v	619	BCR	C23-C24-C25-C26
29	v	619	BCR	C23-C24-C25-C30
29	v	622	BCR	C1-C6-C7-C8
29	v	622	BCR	C5-C6-C7-C8
29	BE	619	BCR	C5-C6-C7-C8
29	BE	619	BCR	C23-C24-C25-C26
29	Bb	101	BCR	C5-C6-C7-C8
29	R	410	BCR	C1-C6-C7-C8
29	R	410	BCR	C5-C6-C7-C8
29	R	410	BCR	C23-C24-C25-C26
29	R	410	BCR	C23-C24-C25-C30
29	1	515	BCR	C23-C24-C25-C26
29	1	515	BCR	C23-C24-C25-C30
29	BD	411	BCR	C1-C6-C7-C8
29	BD	411	BCR	C5-C6-C7-C8
29	BD	411	BCR	C23-C24-C25-C26
29	BF	516	BCR	C5-C6-C7-C8
24	n	613	CLA	C8-C10-C11-C12
24	0	610	CLA	C5-C6-C7-C8
24	BE	605	CLA	C8-C10-C11-C12
27	0	617	LHG	C17-C18-C19-C20
30	C	501	LMG	C17-C18-C19-C20
29	H	101	BCR	C7-C8-C9-C34
29	BD	411	BCR	C7-C8-C9-C34
30	A	412	LMG	C31-C32-C33-C34
25	BU	615	LUT	C7-C8-C9-C10
26	G	617	NEX	C27-C28-C29-C30
26	BJ	617	NEX	C11-C12-C13-C14
28	9	619	XAT	C31-C32-C33-C34
29	AB	313	BCR	C17-C18-C19-C20
29	BE	601	BCR	C17-C18-C19-C20
29	BI	101	BCR	C21-C22-C23-C24
24	b	605	CLA	C8-C10-C11-C12
24	c	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	6	604	CLA	C2C-C3C-CAC-CBC
27	9	618	LHG	C12-C13-C14-C15
29	B	619	BCR	C14-C15-C16-C17
27	6	617	LHG	C30-C31-C32-C33
27	W	201	LHG	C30-C31-C32-C33
32	A1	101	SQD	C32-C33-C34-C35
34	1	517	DGD	C8B-C9B-CAB-CBB
34	1	517	DGD	CBB-CCB-CDB-CEB
23	N	601	CHL	C3-C5-C6-C7
24	g	614	CLA	O2A-C1-C2-C3
24	Au	614	CLA	O2A-C1-C2-C3
24	BQ	614	CLA	O2A-C1-C2-C3
32	BG	406	SQD	O10-C23-O48-C46
32	a	412	SQD	C11-C10-C9-C8
23	G	607	CHL	C16-C17-C18-C19
23	Y	302	CHL	C16-C17-C18-C20
23	Y	310	CHL	C16-C17-C18-C19
23	g	608	CHL	C16-C17-C18-C20
23	Au	601	CHL	C16-C17-C18-C20
23	BB	302	CHL	C16-C17-C18-C20
23	BB	308	CHL	C16-C17-C18-C20
24	s	612	CLA	C6-C7-C8-C10
34	h	102	DGD	C1A-C2A-C3A-C4A
30	C	519	LMG	C18-C19-C20-C21
34	R	401	DGD	C4B-C5B-C6B-C7B
27	G	618	LHG	C13-C14-C15-C16
27	Y	319	LHG	C30-C31-C32-C33
30	C	501	LMG	C30-C31-C32-C33
30	v	623	LMG	C38-C39-C40-C41
30	1	501	LMG	C17-C18-C19-C20
32	BO	102	SQD	C29-C30-C31-C32
34	A	402	DGD	C4E-C5E-C6E-O5E
32	L	103	SQD	C32-C33-C34-C35
27	Y	319	LHG	O6-C4-C5-C6
27	L	102	LHG	O2-C2-C3-O3
27	G	618	LHG	C11-C12-C13-C14
27	d	404	LHG	C34-C35-C36-C37
27	Au	618	LHG	C11-C12-C13-C14
30	BL	101	LMG	C31-C32-C33-C34
23	6	601	CHL	C12-C13-C15-C16
23	N	607	CHL	C12-C13-C15-C16
23	Y	302	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	Y	308	CHL	C12-C13-C15-C16
23	Y	310	CHL	C12-C13-C15-C16
23	g	601	CHL	C11-C12-C13-C15
23	y	308	CHL	C12-C13-C15-C16
23	y	310	CHL	C11-C12-C13-C15
23	y	310	CHL	C12-C13-C15-C16
23	r	605	CHL	C12-C13-C15-C16
23	0	601	CHL	C12-C13-C15-C16
23	Au	607	CHL	C12-C13-C15-C16
23	A2	607	CHL	C12-C13-C15-C16
23	BB	302	CHL	C11-C12-C13-C15
23	BB	308	CHL	C12-C13-C15-C16
23	Ba	308	CHL	C12-C13-C15-C16
23	Ba	310	CHL	C11-C12-C13-C15
23	Ba	310	CHL	C12-C13-C15-C16
23	BU	605	CHL	C12-C13-C15-C16
24	5	602	CLA	C6-C7-C8-C10
24	5	602	CLA	C11-C12-C13-C15
24	B	603	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	G	613	CLA	C6-C7-C8-C10
24	G	613	CLA	C12-C13-C15-C16
24	N	602	CLA	C6-C7-C8-C10
24	N	602	CLA	C11-C12-C13-C15
24	N	610	CLA	C11-C12-C13-C15
24	N	613	CLA	C6-C7-C8-C10
24	Y	314	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
24	n	602	CLA	C11-C12-C13-C15
24	n	610	CLA	C11-C12-C13-C15
24	n	613	CLA	C6-C7-C8-C10
24	y	314	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	c	503	CLA	C11-C10-C8-C7
24	c	511	CLA	C12-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C10
24	r	609	CLA	C6-C7-C8-C10
24	9	602	CLA	C6-C7-C8-C10
24	9	602	CLA	C11-C12-C13-C15
24	v	603	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	v	615	CLA	C11-C12-C13-C15
24	Au	613	CLA	C6-C7-C8-C10
24	Au	613	CLA	C12-C13-C15-C16
24	A2	602	CLA	C6-C7-C8-C10
24	A2	602	CLA	C11-C12-C13-C15
24	A2	610	CLA	C11-C12-C13-C15
24	A2	613	CLA	C6-C7-C8-C10
24	BB	314	CLA	C12-C13-C15-C16
24	BE	616	CLA	C11-C12-C13-C15
24	BE	616	CLA	C12-C13-C15-C16
24	BJ	610	CLA	C11-C12-C13-C15
24	BQ	602	CLA	C11-C12-C13-C15
24	BQ	610	CLA	C11-C12-C13-C15
24	BQ	613	CLA	C6-C7-C8-C10
24	BV	602	CLA	C11-C10-C8-C7
24	Ba	304	CLA	C12-C13-C15-C16
24	Ba	314	CLA	C12-C13-C15-C16
24	1	509	CLA	C11-C10-C8-C7
24	1	510	CLA	C12-C13-C15-C16
24	1	512	CLA	C6-C7-C8-C10
24	BF	503	CLA	C11-C10-C8-C7
24	BF	507	CLA	C11-C12-C13-C15
24	BF	511	CLA	C12-C13-C15-C16
24	BF	513	CLA	C6-C7-C8-C10
24	BU	609	CLA	C6-C7-C8-C10
24	R	405	CLA	O1D-CGD-O2D-CED
24	Ba	313	CLA	O1A-CGA-O2A-C1
24	B	613	CLA	C5-C6-C7-C8
24	BF	506	CLA	C10-C11-C12-C13
26	5	617	NEX	C29-C30-C31-C32
26	y	318	NEX	C9-C10-C11-C12
26	9	617	NEX	C29-C30-C31-C32
28	N	619	XAT	C33-C34-C35-C15
28	n	619	XAT	C29-C30-C31-C32
28	y	301	XAT	C33-C34-C35-C15
28	9	619	XAT	C9-C10-C11-C12
28	A2	619	XAT	C33-C34-C35-C15
28	BB	301	XAT	C13-C14-C15-C35
28	BQ	619	XAT	C13-C14-C15-C35
28	Ba	301	XAT	C33-C34-C35-C15
23	Au	607	CHL	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	A2	611	CLA	C11-C12-C13-C15
27	C	521	LHG	C24-C23-O8-C6
27	L	102	LHG	C13-C14-C15-C16
27	b	624	LHG	C11-C12-C13-C14
32	BD	412	SQD	C11-C10-C9-C8
34	h	102	DGD	C2B-C3B-C4B-C5B
34	c	517	DGD	C8B-C9B-CAB-CBB
30	2	407	LMG	C4-C5-C6-O5
23	5	606	CHL	C2A-CAA-CBA-CGA
23	7	309	CHL	C2A-CAA-CBA-CGA
23	G	609	CHL	C2A-CAA-CBA-CGA
23	N	609	CHL	C2A-CAA-CBA-CGA
23	r	605	CHL	C2A-CAA-CBA-CGA
23	AA	309	CHL	C2A-CAA-CBA-CGA
23	AB	307	CHL	C2A-CAA-CBA-CGA
23	BU	605	CHL	C2A-CAA-CBA-CGA
24	BF	512	CLA	C2A-CAA-CBA-CGA
34	a	401	DGD	C9B-CAB-CBB-CCB
27	c	520	LHG	C8-C7-O7-C5
27	BF	521	LHG	C8-C7-O7-C5
24	s	612	CLA	C5-C6-C7-C8
24	BV	612	CLA	C5-C6-C7-C8
26	7	319	NEX	C20-C13-C14-C15
26	S	616	NEX	C20-C13-C14-C15
26	Y	318	NEX	C11-C10-C9-C19
27	Az	102	LHG	C13-C14-C15-C16
28	N	619	XAT	C20-C13-C14-C15
28	A2	619	XAT	C20-C13-C14-C15
29	B	618	BCR	C20-C21-C22-C37
29	B	619	BCR	C20-C21-C22-C37
29	K	101	BCR	C20-C21-C22-C37
29	b	601	BCR	C35-C13-C14-C15
29	k	101	BCR	C20-C21-C22-C37
29	z	102	BCR	C20-C21-C22-C37
29	v	618	BCR	C20-C21-C22-C37
29	v	622	BCR	C16-C17-C18-C36
29	v	622	BCR	C20-C21-C22-C37
29	Ay	101	BCR	C20-C21-C22-C37
29	BE	601	BCR	C35-C13-C14-C15
29	BE	619	BCR	C16-C17-C18-C36
30	c	518	LMG	C38-C39-C40-C41
30	1	501	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
34	A	402	DGD	C4B-C5B-C6B-C7B
24	A2	613	CLA	C3-C5-C6-C7
24	BB	311	CLA	C3-C5-C6-C7
24	BF	509	CLA	C3-C5-C6-C7
23	6	609	CHL	C10-C11-C12-C13
32	A1	101	SQD	C33-C34-C35-C36
34	A	402	DGD	C8B-C9B-CAB-CBB
34	BD	401	DGD	C9B-CAB-CBB-CCB
23	Au	608	CHL	C16-C17-C18-C19
24	N	611	CLA	C11-C12-C13-C15
24	c	509	CLA	C16-C17-C18-C19
24	r	602	CLA	C11-C12-C13-C14
24	BF	509	CLA	C16-C17-C18-C19
24	BU	602	CLA	C11-C12-C13-C14
23	s	606	CHL	CBA-CGA-O2A-C1
23	BV	606	CHL	CBA-CGA-O2A-C1
24	g	604	CLA	CBA-CGA-O2A-C1
24	A	406	CLA	CBA-CGA-O2A-C1
27	2	406	LHG	C27-C28-C29-C30
27	Au	618	LHG	C34-C35-C36-C37
30	BF	519	LMG	C36-C37-C38-C39
24	G	614	CLA	O2A-C1-C2-C3
23	8	306	CHL	O1D-CGD-O2D-CED
30	A0	201	LMG	C33-C34-C35-C36
32	L	103	SQD	C27-C28-C29-C30
32	l	101	SQD	C27-C28-C29-C30
32	l	102	SQD	C29-C30-C31-C32
32	BD	412	SQD	C19-C20-C21-C22
24	c	508	CLA	C8-C10-C11-C12
24	BF	504	CLA	C13-C15-C16-C17
23	8	306	CHL	CBD-CGD-O2D-CED
23	Au	609	CHL	C2C-C3C-CAC-CBC
30	BF	519	LMG	C18-C19-C20-C21
32	L	103	SQD	C33-C34-C35-C36
34	1	517	DGD	CCA-CDA-CEA-CFA
23	5	606	CHL	CAD-CBD-CGD-O2D
23	5	607	CHL	CAD-CBD-CGD-O2D
23	N	608	CHL	CAD-CBD-CGD-O2D
23	N	609	CHL	CAD-CBD-CGD-O2D
23	g	605	CHL	CAD-CBD-CGD-O2D
23	g	609	CHL	CAD-CBD-CGD-O2D
23	n	606	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	s	605	CHL	CAD-CBD-CGD-O2D
23	y	307	CHL	CAD-CBD-CGD-O2D
23	r	607	CHL	CAD-CBD-CGD-O2D
23	9	606	CHL	CAD-CBD-CGD-O2D
23	A2	608	CHL	CAD-CBD-CGD-O2D
23	A2	609	CHL	CAD-CBD-CGD-O2D
23	BJ	605	CHL	CAD-CBD-CGD-O2D
23	BJ	609	CHL	CAD-CBD-CGD-O2D
23	BQ	606	CHL	CAD-CBD-CGD-O2D
23	BQ	609	CHL	CAD-CBD-CGD-O2D
23	BV	605	CHL	CAD-CBD-CGD-O2D
23	Ba	307	CHL	CAD-CBD-CGD-O2D
23	Ba	309	CHL	CAD-CBD-CGD-O2D
23	Ba	310	CHL	CAD-CBD-CGD-O2D
23	BU	607	CHL	CAD-CBD-CGD-O2D
24	5	614	CLA	CAD-CBD-CGD-O2D
24	7	312	CLA	CAD-CBD-CGD-O2D
24	7	314	CLA	CAD-CBD-CGD-O2D
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	607	CLA	CAD-CBD-CGD-O2D
24	B	609	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	CAD-CBD-CGD-O2D
24	G	603	CLA	CAD-CBD-CGD-O2D
24	G	610	CLA	CAD-CBD-CGD-O2D
24	G	611	CLA	CAD-CBD-CGD-O2D
24	G	613	CLA	CAD-CBD-CGD-O2D
24	N	603	CLA	CAD-CBD-CGD-O2D
24	N	610	CLA	CAD-CBD-CGD-O2D
24	Y	311	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	d	402	CLA	CAD-CBD-CGD-O2D
24	g	613	CLA	CAD-CBD-CGD-O2D
24	n	610	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	a	410	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
24	r	609	CLA	CAD-CBD-CGD-O2D
24	9	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	0	603	CLA	CAD-CBD-CGD-O2D
24	AB	308	CLA	CAD-CBD-CGD-O2D
24	v	602	CLA	CAD-CBD-CGD-O2D
24	v	607	CLA	CAD-CBD-CGD-O2D
24	v	615	CLA	CAD-CBD-CGD-O2D
24	v	616	CLA	CAD-CBD-CGD-O2D
24	Au	603	CLA	CAD-CBD-CGD-O2D
24	Au	610	CLA	CAD-CBD-CGD-O2D
24	Au	611	CLA	CAD-CBD-CGD-O2D
24	Au	613	CLA	CAD-CBD-CGD-O2D
24	A2	603	CLA	CAD-CBD-CGD-O2D
24	A2	614	CLA	CAD-CBD-CGD-O2D
24	BB	311	CLA	CAD-CBD-CGD-O2D
24	BE	608	CLA	CAD-CBD-CGD-O2D
24	BE	614	CLA	CAD-CBD-CGD-O2D
24	BE	617	CLA	CAD-CBD-CGD-O2D
24	BJ	613	CLA	CAD-CBD-CGD-O2D
24	BQ	610	CLA	CAD-CBD-CGD-O2D
24	BV	609	CLA	CAD-CBD-CGD-O2D
24	R	409	CLA	CAD-CBD-CGD-O2D
24	1	506	CLA	CAD-CBD-CGD-O2D
24	1	512	CLA	CAD-CBD-CGD-O2D
24	BD	410	CLA	CAD-CBD-CGD-O2D
24	BF	507	CLA	CAD-CBD-CGD-O2D
26	7	319	NEX	C7-C8-C9-C19
26	S	616	NEX	C7-C8-C9-C19
26	g	617	NEX	C7-C8-C9-C19
26	s	616	NEX	C7-C8-C9-C19
26	AA	319	NEX	C7-C8-C9-C19
26	A6	616	NEX	C7-C8-C9-C19
26	BJ	617	NEX	C7-C8-C9-C19
26	BV	616	NEX	C7-C8-C9-C19
27	C	520	LHG	C6-C5-O7-C7
27	1	520	LHG	C6-C5-O7-C7
27	BF	520	LHG	C6-C5-O7-C7
30	b	621	LMG	C4-C5-C6-O5
30	B	624	LMG	C38-C39-C40-C41
32	A1	101	SQD	C27-C28-C29-C30
23	BB	302	CHL	C13-C15-C16-C17
24	B	605	CLA	C10-C11-C12-C13
24	BE	613	CLA	C13-C15-C16-C17
24	R	404	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	d	404	LHG	C24-C25-C26-C27
29	B	617	BCR	C22-C23-C24-C25
29	B	623	BCR	C22-C23-C24-C25
29	F	101	BCR	C6-C7-C8-C9
29	f	101	BCR	C6-C7-C8-C9
29	v	617	BCR	C22-C23-C24-C25
29	BI	101	BCR	C6-C7-C8-C9
29	BN	101	BCR	C22-C23-C24-C25
24	y	313	CLA	O1A-CGA-O2A-C1
24	BJ	604	CLA	CBA-CGA-O2A-C1
27	2	405	LHG	C24-C23-O8-C6
27	1	521	LHG	C24-C23-O8-C6
32	l	101	SQD	C24-C23-O48-C46
32	BO	101	SQD	C24-C23-O48-C46
24	s	609	CLA	C4-C3-C5-C6
24	A2	611	CLA	C4-C3-C5-C6
24	BE	603	CLA	C16-C17-C18-C20
27	BE	624	LHG	C11-C12-C13-C14
32	BG	406	SQD	C18-C19-C20-C21
34	R	401	DGD	C8B-C9B-CAB-CBB
30	C	501	LMG	O6-C1-O1-C7
30	1	501	LMG	O6-C1-O1-C7
32	2	408	SQD	O5-C1-O6-C44
24	G	602	CLA	C13-C15-C16-C17
24	b	606	CLA	C15-C16-C17-C18
24	BE	602	CLA	C5-C6-C7-C8
27	G	618	LHG	C34-C35-C36-C37
27	5	618	LHG	C7-C8-C9-C10
34	c	517	DGD	C1B-C2B-C3B-C4B
27	y	319	LHG	C4-C5-C6-O8
27	c	519	LHG	C2-C3-O3-P
27	Ba	319	LHG	C4-C5-C6-O8
27	1	520	LHG	C2-C3-O3-P
27	BF	520	LHG	C2-C3-O3-P
30	d	405	LMG	O1-C7-C8-C9
32	R	411	SQD	O6-C44-C45-C46
34	C	516	DGD	C1G-C2G-C3G-O3G
24	6	602	CLA	CBD-CGD-O2D-CED
24	s	610	CLA	O1A-CGA-O2A-C1
24	C	503	CLA	O1A-CGA-O2A-C1
24	v	602	CLA	O1A-CGA-O2A-C1
24	BU	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	CCA-CDA-CEA-CFA
27	5	618	LHG	O6-C4-C5-O7
27	b	622	LHG	O6-C4-C5-O7
27	C	520	LHG	O6-C4-C5-O7
27	c	519	LHG	O6-C4-C5-O7
27	9	618	LHG	O6-C4-C5-O7
27	v	621	LHG	O6-C4-C5-O7
27	BE	622	LHG	O6-C4-C5-O7
27	1	520	LHG	O6-C4-C5-O7
27	BF	520	LHG	O6-C4-C5-O7
23	N	601	CHL	C15-C16-C17-C18
24	b	613	CLA	C13-C15-C16-C17
24	r	610	CLA	O2A-C1-C2-C3
24	BU	610	CLA	O2A-C1-C2-C3
27	c	519	LHG	C15-C16-C17-C18
27	BF	520	LHG	C13-C14-C15-C16
24	B	603	CLA	CBA-CGA-O2A-C1
23	9	601	CHL	C2A-CAA-CBA-CGA
24	BJ	603	CLA	C2A-CAA-CBA-CGA
27	BF	520	LHG	C15-C16-C17-C18
30	A	412	LMG	C33-C34-C35-C36
32	d	406	SQD	C18-C19-C20-C21
24	r	604	CLA	O1A-CGA-O2A-C1
23	G	608	CHL	C16-C17-C18-C19
23	y	308	CHL	C4C-C3C-CAC-CBC
30	c	518	LMG	C36-C37-C38-C39
32	L	103	SQD	C16-C17-C18-C19
24	d	402	CLA	O1D-CGD-O2D-CED
23	7	302	CHL	CHA-CBD-CGD-O1D
23	7	302	CHL	CHA-CBD-CGD-O2D
23	G	605	CHL	CHA-CBD-CGD-O1D
23	G	608	CHL	CHA-CBD-CGD-O1D
23	G	608	CHL	CHA-CBD-CGD-O2D
23	S	605	CHL	CHA-CBD-CGD-O1D
23	S	605	CHL	CHA-CBD-CGD-O2D
23	Y	310	CHL	CHA-CBD-CGD-O2D
23	g	608	CHL	CHA-CBD-CGD-O1D
23	Au	608	CHL	CHA-CBD-CGD-O1D
23	Au	608	CHL	CHA-CBD-CGD-O2D
23	A6	605	CHL	CHA-CBD-CGD-O1D
23	A6	605	CHL	CHA-CBD-CGD-O2D
23	BB	310	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	BJ	608	CHL	CHA-CBD-CGD-O1D
24	5	603	CLA	CHA-CBD-CGD-O1D
24	5	604	CLA	CHA-CBD-CGD-O1D
24	5	612	CLA	CHA-CBD-CGD-O1D
24	6	602	CLA	CHA-CBD-CGD-O1D
24	6	603	CLA	CHA-CBD-CGD-O1D
24	6	604	CLA	CHA-CBD-CGD-O1D
24	6	604	CLA	CHA-CBD-CGD-O2D
24	7	305	CLA	CHA-CBD-CGD-O1D
24	B	605	CLA	CHA-CBD-CGD-O1D
24	B	605	CLA	CHA-CBD-CGD-O2D
24	B	610	CLA	CHA-CBD-CGD-O1D
24	B	610	CLA	CHA-CBD-CGD-O2D
24	B	611	CLA	CHA-CBD-CGD-O1D
24	B	611	CLA	CHA-CBD-CGD-O2D
24	B	612	CLA	CHA-CBD-CGD-O1D
24	B	612	CLA	CHA-CBD-CGD-O2D
24	G	602	CLA	CHA-CBD-CGD-O1D
24	G	602	CLA	CHA-CBD-CGD-O2D
24	G	612	CLA	CHA-CBD-CGD-O1D
24	G	612	CLA	CHA-CBD-CGD-O2D
24	N	602	CLA	CHA-CBD-CGD-O1D
24	N	604	CLA	CHA-CBD-CGD-O1D
24	N	612	CLA	CHA-CBD-CGD-O1D
24	N	612	CLA	CHA-CBD-CGD-O2D
24	Y	303	CLA	CHA-CBD-CGD-O1D
24	Y	303	CLA	CHA-CBD-CGD-O2D
24	Y	305	CLA	CHA-CBD-CGD-O1D
24	Y	305	CLA	CHA-CBD-CGD-O2D
24	b	611	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	612	CLA	CHA-CBD-CGD-O1D
24	b	612	CLA	CHA-CBD-CGD-O2D
24	g	602	CLA	CHA-CBD-CGD-O1D
24	g	602	CLA	CHA-CBD-CGD-O2D
24	g	604	CLA	CHA-CBD-CGD-O1D
24	g	604	CLA	CHA-CBD-CGD-O2D
24	g	612	CLA	CHA-CBD-CGD-O1D
24	s	604	CLA	CHA-CBD-CGD-O1D
24	y	303	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	511	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	9	603	CLA	CHA-CBD-CGD-O1D
24	9	604	CLA	CHA-CBD-CGD-O1D
24	9	612	CLA	CHA-CBD-CGD-O1D
24	9	612	CLA	CHA-CBD-CGD-O2D
24	0	602	CLA	CHA-CBD-CGD-O1D
24	AA	305	CLA	CHA-CBD-CGD-O1D
24	v	605	CLA	CHA-CBD-CGD-O1D
24	v	605	CLA	CHA-CBD-CGD-O2D
24	v	610	CLA	CHA-CBD-CGD-O1D
24	v	610	CLA	CHA-CBD-CGD-O2D
24	v	611	CLA	CHA-CBD-CGD-O1D
24	v	612	CLA	CHA-CBD-CGD-O1D
24	v	612	CLA	CHA-CBD-CGD-O2D
24	Au	602	CLA	CHA-CBD-CGD-O1D
24	Au	602	CLA	CHA-CBD-CGD-O2D
24	Au	612	CLA	CHA-CBD-CGD-O1D
24	Au	612	CLA	CHA-CBD-CGD-O2D
24	A2	602	CLA	CHA-CBD-CGD-O1D
24	A2	604	CLA	CHA-CBD-CGD-O1D
24	A2	612	CLA	CHA-CBD-CGD-O1D
24	A2	612	CLA	CHA-CBD-CGD-O2D
24	BB	303	CLA	CHA-CBD-CGD-O1D
24	BB	303	CLA	CHA-CBD-CGD-O2D
24	BB	305	CLA	CHA-CBD-CGD-O1D
24	BB	305	CLA	CHA-CBD-CGD-O2D
24	BE	606	CLA	CHA-CBD-CGD-O1D
24	BE	611	CLA	CHA-CBD-CGD-O1D
24	BE	611	CLA	CHA-CBD-CGD-O2D
24	BE	612	CLA	CHA-CBD-CGD-O1D
24	BE	613	CLA	CHA-CBD-CGD-O1D
24	BJ	602	CLA	CHA-CBD-CGD-O1D
24	BJ	602	CLA	CHA-CBD-CGD-O2D
24	BJ	604	CLA	CHA-CBD-CGD-O1D
24	BJ	604	CLA	CHA-CBD-CGD-O2D
24	BJ	612	CLA	CHA-CBD-CGD-O1D
24	Ba	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	1	508	CLA	CHA-CBD-CGD-O1D
24	1	509	CLA	CHA-CBD-CGD-O1D
24	BF	502	CLA	CHA-CBD-CGD-O1D
24	BF	502	CLA	CHA-CBD-CGD-O2D
24	BF	509	CLA	CHA-CBD-CGD-O1D
24	BF	512	CLA	CHA-CBD-CGD-O1D
24	BU	604	CLA	CHA-CBD-CGD-O1D
29	v	622	BCR	C19-C20-C21-C22
32	BO	101	SQD	C27-C28-C29-C30
24	d	401	CLA	C3-C5-C6-C7
23	9	607	CHL	O1A-CGA-O2A-C1
24	Au	611	CLA	O1A-CGA-O2A-C1
24	BV	610	CLA	O1A-CGA-O2A-C1
27	1	521	LHG	C25-C26-C27-C28
24	n	614	CLA	O2A-C1-C2-C3
24	A2	614	CLA	O2A-C1-C2-C3
26	7	319	NEX	C12-C13-C14-C15
26	S	616	NEX	C28-C29-C30-C31
26	BQ	617	NEX	C11-C10-C9-C8
29	4	101	BCR	C12-C13-C14-C15
27	w	201	LHG	C30-C31-C32-C33
30	BF	519	LMG	C38-C39-C40-C41
32	a	412	SQD	C30-C31-C32-C33
32	A1	101	SQD	C16-C17-C18-C19
27	B	621	LHG	O7-C5-C6-O8
27	b	622	LHG	O7-C5-C6-O8
27	v	621	LHG	O7-C5-C6-O8
27	BE	622	LHG	O7-C5-C6-O8
34	A	402	DGD	O2G-C2G-C3G-O3G
34	R	401	DGD	O2G-C2G-C3G-O3G
34	1	516	DGD	O2G-C2G-C3G-O3G
27	n	618	LHG	C29-C30-C31-C32
27	Au	618	LHG	C33-C34-C35-C36
32	BD	412	SQD	C30-C31-C32-C33
34	h	102	DGD	C4B-C5B-C6B-C7B
27	9	618	LHG	C7-C8-C9-C10
24	g	602	CLA	C13-C15-C16-C17
24	A	405	CLA	C13-C15-C16-C17
24	B	602	CLA	O1A-CGA-O2A-C1
24	c	503	CLA	O1A-CGA-O2A-C1
24	BJ	604	CLA	O1A-CGA-O2A-C1
24	BV	609	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	1	503	CLA	O1A-CGA-O2A-C1
24	BD	406	CLA	O1A-CGA-O2A-C1
27	D	404	LHG	C34-C35-C36-C37
27	N	618	LHG	C13-C14-C15-C16
27	BB	319	LHG	C25-C26-C27-C28
27	BQ	618	LHG	C29-C30-C31-C32
24	B	601	CLA	C16-C17-C18-C20
24	C	511	CLA	C16-C17-C18-C19
24	C	511	CLA	C16-C17-C18-C20
23	AB	306	CHL	O1D-CGD-O2D-CED
24	2	403	CLA	O1D-CGD-O2D-CED
30	c	518	LMG	C18-C19-C20-C21
30	2	407	LMG	C15-C16-C17-C18
24	b	602	CLA	C5-C6-C7-C8
24	BE	606	CLA	C15-C16-C17-C18
23	7	308	CHL	C4-C3-C5-C6
24	B	609	CLA	C4-C3-C5-C6
24	BE	608	CLA	C4-C3-C5-C6
31	D	403	PL9	C20-C19-C21-C22
27	Y	319	LHG	C32-C33-C34-C35
27	BY	201	LHG	C30-C31-C32-C33
32	d	406	SQD	O10-C23-O48-C46
23	5	607	CHL	C2-C3-C5-C6
23	n	601	CHL	C14-C13-C15-C16
23	y	308	CHL	C14-C13-C15-C16
23	9	609	CHL	C11-C12-C13-C14
23	Ba	308	CHL	C14-C13-C15-C16
24	Y	314	CLA	C14-C13-C15-C16
24	C	512	CLA	C6-C7-C8-C9
24	c	511	CLA	C14-C13-C15-C16
24	BB	314	CLA	C14-C13-C15-C16
24	1	512	CLA	C6-C7-C8-C9
24	BF	511	CLA	C14-C13-C15-C16
27	2	406	LHG	C34-C35-C36-C37
27	A2	618	LHG	C13-C14-C15-C16
30	B	620	LMG	C31-C32-C33-C34
30	D	405	LMG	C15-C16-C17-C18
24	g	604	CLA	O1A-CGA-O2A-C1
32	D	406	SQD	C4-C5-C6-S
32	d	406	SQD	C4-C5-C6-S
32	BG	406	SQD	C4-C5-C6-S
30	D	405	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	B	624	LMG	C35-C36-C37-C38
23	6	608	CHL	C2A-CAA-CBA-CGA
23	0	608	CHL	C2A-CAA-CBA-CGA
23	Au	609	CHL	C2A-CAA-CBA-CGA
23	A6	607	CHL	C2A-CAA-CBA-CGA
24	g	603	CLA	C2A-CAA-CBA-CGA
24	y	314	CLA	C2A-CAA-CBA-CGA
24	v	603	CLA	C2A-CAA-CBA-CGA
27	G	618	LHG	C33-C34-C35-C36
34	BF	518	DGD	CCA-CDA-CEA-CFA
23	BV	606	CHL	O1A-CGA-O2A-C1
25	BJ	615	LUT	C7-C8-C9-C19
26	9	617	NEX	C11-C12-C13-C20
26	Au	617	NEX	C27-C28-C29-C39
26	Au	617	NEX	C31-C32-C33-C40
30	D	405	LMG	C17-C18-C19-C20
34	BK	102	DGD	C2B-C3B-C4B-C5B
26	5	617	NEX	C11-C12-C13-C14
26	g	617	NEX	C11-C12-C13-C14
28	BQ	619	XAT	C31-C32-C33-C34
29	B	618	BCR	C7-C8-C9-C10
29	F	101	BCR	C21-C22-C23-C24
29	v	618	BCR	C7-C8-C9-C10
24	B	601	CLA	C3-C5-C6-C7
24	b	602	CLA	C3-C5-C6-C7
24	v	601	CLA	C3-C5-C6-C7
24	BE	602	CLA	C3-C5-C6-C7
30	d	405	LMG	C17-C18-C19-C20
34	H	102	DGD	C4B-C5B-C6B-C7B
34	BK	102	DGD	C4B-C5B-C6B-C7B
23	7	307	CHL	C1A-C2A-CAA-CBA
23	N	609	CHL	C1A-C2A-CAA-CBA
23	g	605	CHL	C1A-C2A-CAA-CBA
23	n	606	CHL	C1A-C2A-CAA-CBA
23	BJ	605	CHL	C1A-C2A-CAA-CBA
24	B	606	CLA	C1A-C2A-CAA-CBA
24	I	102	CLA	C1A-C2A-CAA-CBA
24	N	604	CLA	C1A-C2A-CAA-CBA
24	Y	303	CLA	C1A-C2A-CAA-CBA
24	y	303	CLA	C1A-C2A-CAA-CBA
24	v	606	CLA	C1A-C2A-CAA-CBA
24	Ba	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	7	304	CLA	C6-C7-C8-C9
24	AA	304	CLA	C6-C7-C8-C9
24	b	606	CLA	C13-C15-C16-C17
24	BF	508	CLA	C8-C10-C11-C12
23	S	606	CHL	CBA-CGA-O2A-C1
23	A6	606	CHL	CBA-CGA-O2A-C1
27	A2	618	LHG	C24-C23-O8-C6
27	BE	622	LHG	C14-C15-C16-C17
30	v	623	LMG	C35-C36-C37-C38
30	BF	501	LMG	C35-C36-C37-C38
34	C	517	DGD	C8B-C9B-CAB-CBB
28	n	619	XAT	C33-C34-C35-C15
29	b	601	BCR	C19-C20-C21-C22
27	L	102	LHG	C3-O3-P-O6
27	d	404	LHG	C4-O6-P-O3
27	Az	102	LHG	C3-O3-P-O6
27	BE	624	LHG	C3-O3-P-O6
27	A2	618	LHG	C31-C32-C33-C34
30	BE	621	LMG	C21-C22-C23-C24
30	C	519	LMG	C19-C20-C21-C22
30	1	519	LMG	C19-C20-C21-C22
32	A1	101	SQD	C29-C30-C31-C32
23	n	607	CHL	C4-C3-C5-C6
23	BQ	607	CHL	C4-C3-C5-C6
27	5	618	LHG	C2-C3-O3-P
27	d	404	LHG	C2-C3-O3-P
27	C	520	LHG	C2-C3-O3-P
27	9	618	LHG	C2-C3-O3-P
27	BG	404	LHG	C2-C3-O3-P
24	Y	314	CLA	C2-C3-C5-C6
34	BF	518	DGD	C5B-C6B-C7B-C8B
24	A	406	CLA	O1A-CGA-O2A-C1
27	9	618	LHG	O10-C23-O8-C6
32	l	101	SQD	O10-C23-O48-C46
32	BO	101	SQD	O10-C23-O48-C46
23	7	309	CHL	C4B-C3B-CAB-CBB
23	8	305	CHL	C4B-C3B-CAB-CBB
23	S	607	CHL	C4B-C3B-CAB-CBB
23	AB	305	CHL	C4B-C3B-CAB-CBB
23	A6	607	CHL	C4B-C3B-CAB-CBB
24	5	603	CLA	C4B-C3B-CAB-CBB
24	5	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	6	612	CLA	C4B-C3B-CAB-CBB
24	6	614	CLA	C4B-C3B-CAB-CBB
24	7	304	CLA	C4B-C3B-CAB-CBB
24	8	302	CLA	C4B-C3B-CAB-CBB
24	8	309	CLA	C4B-C3B-CAB-CBB
24	G	603	CLA	C4B-C3B-CAB-CBB
24	G	612	CLA	C4B-C3B-CAB-CBB
24	S	608	CLA	C4B-C3B-CAB-CBB
24	Y	304	CLA	C4B-C3B-CAB-CBB
24	Y	312	CLA	C4B-C3B-CAB-CBB
24	Y	313	CLA	C4B-C3B-CAB-CBB
24	g	603	CLA	C4B-C3B-CAB-CBB
24	g	611	CLA	C4B-C3B-CAB-CBB
24	n	603	CLA	C4B-C3B-CAB-CBB
24	n	611	CLA	C4B-C3B-CAB-CBB
24	s	610	CLA	C4B-C3B-CAB-CBB
24	y	312	CLA	C4B-C3B-CAB-CBB
24	A	407	CLA	C4B-C3B-CAB-CBB
24	a	407	CLA	C4B-C3B-CAB-CBB
24	r	601	CLA	C4B-C3B-CAB-CBB
24	r	614	CLA	C4B-C3B-CAB-CBB
24	9	611	CLA	C4B-C3B-CAB-CBB
24	9	612	CLA	C4B-C3B-CAB-CBB
24	0	614	CLA	C4B-C3B-CAB-CBB
24	AA	304	CLA	C4B-C3B-CAB-CBB
24	AB	302	CLA	C4B-C3B-CAB-CBB
24	AB	309	CLA	C4B-C3B-CAB-CBB
24	Au	603	CLA	C4B-C3B-CAB-CBB
24	Au	612	CLA	C4B-C3B-CAB-CBB
24	A6	608	CLA	C4B-C3B-CAB-CBB
24	BB	304	CLA	C4B-C3B-CAB-CBB
24	BB	312	CLA	C4B-C3B-CAB-CBB
24	BB	313	CLA	C4B-C3B-CAB-CBB
24	BJ	611	CLA	C4B-C3B-CAB-CBB
24	BQ	603	CLA	C4B-C3B-CAB-CBB
24	BQ	611	CLA	C4B-C3B-CAB-CBB
24	BV	610	CLA	C4B-C3B-CAB-CBB
24	Ba	312	CLA	C4B-C3B-CAB-CBB
24	R	406	CLA	C4B-C3B-CAB-CBB
24	BD	407	CLA	C4B-C3B-CAB-CBB
24	BU	608	CLA	C4B-C3B-CAB-CBB
24	BU	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	B	622	LHG	C4-O6-P-O5
27	D	404	LHG	C3-O3-P-O4
27	b	622	LHG	C4-O6-P-O5
27	d	404	LHG	C3-O3-P-O4
27	n	618	LHG	C3-O3-P-O5
27	C	520	LHG	C3-O3-P-O4
27	C	521	LHG	C3-O3-P-O5
27	c	520	LHG	C3-O3-P-O5
27	2	406	LHG	C3-O3-P-O4
27	BE	622	LHG	C4-O6-P-O5
27	BG	404	LHG	C3-O3-P-O4
27	BQ	618	LHG	C3-O3-P-O5
27	1	520	LHG	C3-O3-P-O4
27	1	521	LHG	C3-O3-P-O5
27	BF	521	LHG	C3-O3-P-O5
23	G	601	CHL	C16-C17-C18-C19
23	Y	302	CHL	C16-C17-C18-C19
23	Au	601	CHL	C16-C17-C18-C19
23	A2	609	CHL	C16-C17-C18-C20
23	BB	302	CHL	C16-C17-C18-C19
23	Ba	302	CHL	C16-C17-C18-C19
24	c	503	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
24	v	601	CLA	C16-C17-C18-C20
24	BF	503	CLA	C16-C17-C18-C20
24	BF	512	CLA	C16-C17-C18-C19
27	BJ	618	LHG	C24-C25-C26-C27
34	c	517	DGD	C5B-C6B-C7B-C8B
34	Av	102	DGD	C4B-C5B-C6B-C7B
24	r	611	CLA	O2A-C1-C2-C3
24	BU	611	CLA	O2A-C1-C2-C3
24	2	402	CLA	C13-C15-C16-C17
24	v	603	CLA	CBA-CGA-O2A-C1
24	BQ	602	CLA	CBA-CGA-O2A-C1
27	N	618	LHG	C24-C23-O8-C6
27	5	618	LHG	O6-C4-C5-C6
27	6	617	LHG	O6-C4-C5-C6
27	y	319	LHG	O6-C4-C5-C6
27	9	618	LHG	O6-C4-C5-C6
27	0	617	LHG	O6-C4-C5-C6
27	Ba	319	LHG	O6-C4-C5-C6
30	b	621	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	b	622	LHG	C14-C15-C16-C17
24	BE	606	CLA	C13-C15-C16-C17
24	C	507	CLA	C2A-CAA-CBA-CGA
24	c	503	CLA	C2A-CAA-CBA-CGA
24	Ba	314	CLA	C2A-CAA-CBA-CGA
24	s	602	CLA	C3-C5-C6-C7
24	c	508	CLA	C3-C5-C6-C7
23	A2	601	CHL	C15-C16-C17-C18
23	7	310	CHL	C4C-C3C-CAC-CBC
27	C	521	LHG	C25-C26-C27-C28
30	b	621	LMG	C37-C38-C39-C40
30	c	501	LMG	C30-C31-C32-C33
30	c	501	LMG	C35-C36-C37-C38
30	2	407	LMG	C17-C18-C19-C20
23	s	606	CHL	O1A-CGA-O2A-C1
27	C	521	LHG	C8-C7-O7-C5
24	N	614	CLA	O2A-C1-C2-C3
23	N	609	CHL	C16-C17-C18-C20
27	g	618	LHG	C17-C18-C19-C20
32	L	103	SQD	C29-C30-C31-C32
23	G	605	CHL	CAD-CBD-CGD-O1D
23	G	608	CHL	CAD-CBD-CGD-O1D
23	S	605	CHL	CAD-CBD-CGD-O1D
23	g	608	CHL	CAD-CBD-CGD-O1D
23	9	607	CHL	CAD-CBD-CGD-O1D
23	Au	605	CHL	CAD-CBD-CGD-O1D
23	Au	608	CHL	CAD-CBD-CGD-O1D
23	A6	605	CHL	CAD-CBD-CGD-O1D
23	BJ	608	CHL	CAD-CBD-CGD-O1D
24	5	603	CLA	CAD-CBD-CGD-O1D
24	5	604	CLA	CAD-CBD-CGD-O1D
24	6	604	CLA	CAD-CBD-CGD-O1D
24	B	604	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	612	CLA	CAD-CBD-CGD-O1D
24	I	102	CLA	CAD-CBD-CGD-O1D
24	N	612	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	g	611	CLA	CAD-CBD-CGD-O1D
24	n	612	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	CAD-CBD-CGD-O1D
24	9	604	CLA	CAD-CBD-CGD-O1D
24	0	604	CLA	CAD-CBD-CGD-O1D
24	v	604	CLA	CAD-CBD-CGD-O1D
24	v	605	CLA	CAD-CBD-CGD-O1D
24	v	612	CLA	CAD-CBD-CGD-O1D
24	Aw	102	CLA	CAD-CBD-CGD-O1D
24	A2	612	CLA	CAD-CBD-CGD-O1D
24	BE	605	CLA	CAD-CBD-CGD-O1D
24	BE	606	CLA	CAD-CBD-CGD-O1D
24	BJ	611	CLA	CAD-CBD-CGD-O1D
24	BQ	612	CLA	CAD-CBD-CGD-O1D
24	1	502	CLA	CAD-CBD-CGD-O1D
24	BF	502	CLA	CAD-CBD-CGD-O1D
32	L	101	SQD	O5-C5-C6-S
32	L	103	SQD	O5-C5-C6-S
32	A1	101	SQD	O5-C5-C6-S
23	N	609	CHL	CBD-CGD-O2D-CED
23	AB	306	CHL	CBD-CGD-O2D-CED
30	BG	405	LMG	C17-C18-C19-C20
32	l	102	SQD	C24-C25-C26-C27
32	BO	102	SQD	C24-C25-C26-C27
24	B	603	CLA	O1A-CGA-O2A-C1
34	c	517	DGD	CCA-CDA-CEA-CFA
23	Y	302	CHL	C13-C15-C16-C17
24	g	612	CLA	C5-C6-C7-C8
27	A2	618	LHG	C15-C16-C17-C18
34	BF	518	DGD	C1B-C2B-C3B-C4B
30	BF	501	LMG	C30-C31-C32-C33
24	R	405	CLA	CBA-CGA-O2A-C1
27	L	102	LHG	C1-C2-C3-O3
27	BJ	618	LHG	C17-C18-C19-C20
27	1	521	LHG	C10-C11-C12-C13
30	i	101	LMG	C33-C34-C35-C36
32	BO	101	SQD	C16-C17-C18-C19
34	C	517	DGD	CBB-CCB-CDB-CEB
24	S	612	CLA	C6-C7-C8-C10
23	N	607	CHL	C4-C3-C5-C6
24	BB	313	CLA	C4-C3-C5-C6
31	BG	403	PL9	C20-C19-C21-C22
23	5	609	CHL	C11-C12-C13-C15
23	6	608	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	7	308	CHL	C2-C3-C5-C6
23	G	601	CHL	C11-C12-C13-C15
23	N	601	CHL	C11-C12-C13-C15
23	Y	309	CHL	C11-C12-C13-C15
23	Y	310	CHL	C11-C12-C13-C15
23	n	601	CHL	C12-C13-C15-C16
23	n	607	CHL	C12-C13-C15-C16
23	y	309	CHL	C11-C12-C13-C15
23	9	607	CHL	C2-C3-C5-C6
23	9	609	CHL	C11-C12-C13-C15
23	0	601	CHL	C3A-C2A-CAA-CBA
23	0	608	CHL	C3A-C2A-CAA-CBA
23	Au	601	CHL	C11-C12-C13-C15
23	A2	601	CHL	C11-C12-C13-C15
23	BB	302	CHL	C3A-C2A-CAA-CBA
23	BB	309	CHL	C11-C12-C13-C15
23	BB	310	CHL	C11-C12-C13-C15
23	BQ	607	CHL	C12-C13-C15-C16
23	Ba	309	CHL	C11-C12-C13-C15
24	B	606	CLA	C12-C13-C15-C16
24	B	614	CLA	C12-C13-C15-C16
24	B	616	CLA	C6-C7-C8-C10
24	D	401	CLA	C6-C7-C8-C10
24	Y	303	CLA	C11-C10-C8-C7
24	b	607	CLA	C12-C13-C15-C16
24	b	608	CLA	C11-C10-C8-C7
24	b	613	CLA	C11-C10-C8-C7
24	b	615	CLA	C12-C13-C15-C16
24	b	617	CLA	C6-C7-C8-C10
24	d	401	CLA	C6-C7-C8-C10
24	d	401	CLA	C11-C10-C8-C7
24	d	402	CLA	C11-C12-C13-C15
24	n	602	CLA	C6-C7-C8-C10
24	n	604	CLA	C3A-C2A-CAA-CBA
24	y	304	CLA	C12-C13-C15-C16
24	C	512	CLA	C6-C7-C8-C10
24	c	511	CLA	C11-C10-C8-C7
24	r	602	CLA	C6-C7-C8-C10
24	v	607	CLA	C11-C10-C8-C7
24	v	614	CLA	C12-C13-C15-C16
24	v	616	CLA	C6-C7-C8-C10
24	2	402	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	Au	610	CLA	C11-C10-C8-C7
24	BB	303	CLA	C11-C10-C8-C7
24	BB	304	CLA	C12-C13-C15-C16
24	BB	314	CLA	C2-C3-C5-C6
24	BE	607	CLA	C12-C13-C15-C16
24	BE	608	CLA	C11-C10-C8-C7
24	BE	613	CLA	C11-C10-C8-C7
24	BE	615	CLA	C12-C13-C15-C16
24	BE	617	CLA	C6-C7-C8-C10
24	BG	401	CLA	C6-C7-C8-C10
24	BG	401	CLA	C11-C10-C8-C7
24	BG	402	CLA	C11-C12-C13-C15
24	BQ	602	CLA	C6-C7-C8-C10
24	BF	511	CLA	C11-C10-C8-C7
24	BU	602	CLA	C6-C7-C8-C10
27	N	618	LHG	C30-C31-C32-C33
27	N	618	LHG	C31-C32-C33-C34
30	v	620	LMG	C31-C32-C33-C34
24	Au	602	CLA	C13-C15-C16-C17
24	BE	603	CLA	C8-C10-C11-C12
27	g	618	LHG	C24-C25-C26-C27
27	n	618	LHG	C30-C31-C32-C33
27	N	618	LHG	C15-C16-C17-C18
24	5	602	CLA	C8-C10-C11-C12
24	1	505	CLA	C5-C6-C7-C8
27	1	521	LHG	C8-C7-O7-C5
27	9	618	LHG	C11-C10-C9-C8
23	A6	606	CHL	O1A-CGA-O2A-C1
23	0	609	CHL	C10-C11-C12-C13
23	BU	605	CHL	C10-C11-C12-C13
23	r	607	CHL	C2C-C3C-CAC-CBC
27	y	319	LHG	C34-C35-C36-C37
30	BL	101	LMG	C33-C34-C35-C36
30	1	501	LMG	C38-C39-C40-C41
24	BE	612	CLA	C10-C11-C12-C13
23	BJ	601	CHL	C16-C17-C18-C19
23	BJ	608	CHL	C16-C17-C18-C19
24	b	603	CLA	C16-C17-C18-C20
30	C	501	LMG	C38-C39-C40-C41
27	D	404	LHG	C7-C8-C9-C10
34	C	517	DGD	C1B-C2B-C3B-C4B
34	1	517	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
24	BJ	612	CLA	C5-C6-C7-C8
23	6	608	CHL	C1C-C2C-CMC-OMC
23	7	310	CHL	C1C-C2C-CMC-OMC
23	G	608	CHL	C1C-C2C-CMC-OMC
23	N	601	CHL	C1C-C2C-CMC-OMC
23	N	605	CHL	C1C-C2C-CMC-OMC
23	N	608	CHL	C1C-C2C-CMC-OMC
23	n	608	CHL	C1C-C2C-CMC-OMC
23	n	609	CHL	C1C-C2C-CMC-OMC
23	y	309	CHL	C1C-C2C-CMC-OMC
23	y	310	CHL	C1C-C2C-CMC-OMC
23	r	606	CHL	C1C-C2C-CMC-OMC
23	9	609	CHL	C1C-C2C-CMC-OMC
23	0	608	CHL	C1C-C2C-CMC-OMC
23	AA	308	CHL	C1C-C2C-CMC-OMC
23	AB	304	CHL	C1C-C2C-CMC-OMC
23	Au	601	CHL	C1C-C2C-CMC-OMC
23	Au	608	CHL	C1C-C2C-CMC-OMC
23	A2	601	CHL	C1C-C2C-CMC-OMC
23	A2	605	CHL	C1C-C2C-CMC-OMC
23	A2	608	CHL	C1C-C2C-CMC-OMC
23	BQ	608	CHL	C1C-C2C-CMC-OMC
23	Ba	309	CHL	C1C-C2C-CMC-OMC
23	Ba	310	CHL	C1C-C2C-CMC-OMC
23	BU	606	CHL	C1C-C2C-CMC-OMC
23	BU	613	CHL	C1C-C2C-CMC-OMC
27	Y	319	LHG	C25-C26-C27-C28
27	b	623	LHG	C33-C34-C35-C36
27	C	521	LHG	C4-C5-C6-O8
27	c	519	LHG	C29-C30-C31-C32
27	1	521	LHG	C4-C5-C6-O8
30	i	101	LMG	O1-C7-C8-C9
30	A	412	LMG	O1-C7-C8-C9
30	A0	201	LMG	O1-C7-C8-C9
30	A0	201	LMG	C7-C8-C9-O8
30	BL	101	LMG	O1-C7-C8-C9
34	c	517	DGD	C1G-C2G-C3G-O3G
34	1	516	DGD	C1G-C2G-C3G-O3G
34	BF	518	DGD	C1G-C2G-C3G-O3G
30	i	101	LMG	O1-C7-C8-O7
30	c	518	LMG	O7-C8-C9-O8
30	A0	201	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
30	BF	519	LMG	O7-C8-C9-O8
34	A	402	DGD	O1G-C1G-C2G-O2G
34	c	517	DGD	O2G-C2G-C3G-O3G
34	R	401	DGD	O1G-C1G-C2G-O2G
34	BF	518	DGD	O2G-C2G-C3G-O3G
27	2	405	LHG	C33-C34-C35-C36
27	BB	319	LHG	C32-C33-C34-C35
27	Ba	319	LHG	C34-C35-C36-C37
24	D	402	CLA	O1D-CGD-O2D-CED
23	S	606	CHL	O1A-CGA-O2A-C1
24	BQ	602	CLA	O1A-CGA-O2A-C1
27	5	618	LHG	O10-C23-O8-C6
30	BE	621	LMG	O10-C28-O8-C9
27	v	621	LHG	C31-C32-C33-C34
27	BQ	618	LHG	C30-C31-C32-C33
30	v	620	LMG	C37-C38-C39-C40
24	b	602	CLA	C16-C17-C18-C19
24	BE	602	CLA	C16-C17-C18-C19
24	c	504	CLA	C13-C15-C16-C17
24	v	602	CLA	C15-C16-C17-C18
24	c	509	CLA	C3-C5-C6-C7
24	BF	508	CLA	C3-C5-C6-C7
23	g	607	CHL	C10-C11-C12-C13
23	y	308	CHL	C10-C11-C12-C13
23	r	605	CHL	C10-C11-C12-C13
23	BJ	607	CHL	C10-C11-C12-C13
23	Ba	308	CHL	C10-C11-C12-C13
24	v	603	CLA	O1A-CGA-O2A-C1
23	BQ	609	CHL	C13-C15-C16-C17
23	A2	607	CHL	C4-C3-C5-C6
24	Y	313	CLA	C4-C3-C5-C6
24	BF	503	CLA	CBA-CGA-O2A-C1
27	B	622	LHG	C24-C23-O8-C6
30	BG	405	LMG	C11-C12-C13-C14
32	BD	412	SQD	O47-C7-C8-C9
27	B	622	LHG	C24-C25-C26-C27
30	C	519	LMG	C38-C39-C40-C41
32	l	101	SQD	C16-C17-C18-C19
24	B	601	CLA	C5-C6-C7-C8
24	v	601	CLA	C5-C6-C7-C8
24	BQ	611	CLA	C10-C11-C12-C13
23	5	609	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	N	607	CHL	C14-C13-C15-C16
23	Y	302	CHL	C11-C12-C13-C14
23	Y	308	CHL	C14-C13-C15-C16
23	g	607	CHL	C14-C13-C15-C16
23	n	607	CHL	C14-C13-C15-C16
23	y	302	CHL	C11-C12-C13-C14
23	r	605	CHL	C14-C13-C15-C16
23	A2	607	CHL	C14-C13-C15-C16
23	BB	302	CHL	C11-C12-C13-C14
23	BB	308	CHL	C14-C13-C15-C16
23	BQ	607	CHL	C14-C13-C15-C16
23	Ba	302	CHL	C11-C12-C13-C14
23	Ba	310	CHL	C11-C12-C13-C14
23	BU	605	CHL	C14-C13-C15-C16
24	B	612	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	G	610	CLA	C11-C12-C13-C14
24	G	613	CLA	C6-C7-C8-C9
24	N	602	CLA	C11-C12-C13-C14
24	g	602	CLA	C14-C13-C15-C16
24	y	314	CLA	C11-C12-C13-C14
24	v	612	CLA	C11-C10-C8-C9
24	Au	613	CLA	C6-C7-C8-C9
24	A2	602	CLA	C11-C10-C8-C9
24	A2	602	CLA	C11-C12-C13-C14
24	BB	312	CLA	C11-C10-C8-C9
24	BE	603	CLA	C14-C13-C15-C16
24	BJ	602	CLA	C14-C13-C15-C16
24	Ba	314	CLA	C11-C12-C13-C14
29	K	101	BCR	C22-C23-C24-C25
29	k	101	BCR	C22-C23-C24-C25
29	Ay	101	BCR	C22-C23-C24-C25
27	B	622	LHG	C33-C34-C35-C36
27	C	521	LHG	C10-C11-C12-C13
24	C	503	CLA	C3-C5-C6-C7
23	g	608	CHL	C16-C17-C18-C19
24	B	601	CLA	C16-C17-C18-C19
24	b	603	CLA	C16-C17-C18-C19
24	BF	512	CLA	C16-C17-C18-C20
30	1	519	LMG	C38-C39-C40-C41
34	C	516	DGD	O6D-C1D-O3G-C3G
27	B	621	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	d	405	LMG	C11-C12-C13-C14
24	6	613	CLA	O1A-CGA-O2A-C1
24	R	405	CLA	O1A-CGA-O2A-C1
24	c	508	CLA	C2A-CAA-CBA-CGA
32	a	412	SQD	O47-C7-C8-C9
24	n	611	CLA	C10-C11-C12-C13
27	B	621	LHG	C29-C30-C31-C32
27	C	520	LHG	C9-C10-C11-C12
28	5	619	XAT	C33-C34-C35-C15
28	BQ	619	XAT	C29-C30-C31-C32
25	g	615	LUT	C7-C8-C9-C19
25	AA	316	LUT	C7-C8-C9-C19
28	n	619	XAT	C31-C32-C33-C40
24	B	602	CLA	C15-C16-C17-C18
30	b	621	LMG	O10-C28-O8-C9
27	5	618	LHG	C11-C10-C9-C8
24	c	512	CLA	C16-C17-C18-C20
24	A6	612	CLA	C6-C7-C8-C10
27	b	623	LHG	C24-C25-C26-C27
27	Ba	319	LHG	C30-C31-C32-C33
25	r	615	LUT	C7-C8-C9-C10
29	4	101	BCR	C21-C22-C23-C24
24	D	401	CLA	C13-C15-C16-C17
24	v	602	CLA	C8-C10-C11-C12
24	BJ	602	CLA	C13-C15-C16-C17
34	BF	518	DGD	CBB-CCB-CDB-CEB
24	5	604	CLA	C2B-C3B-CAB-CBB
24	5	611	CLA	C2B-C3B-CAB-CBB
24	6	602	CLA	C2B-C3B-CAB-CBB
24	6	612	CLA	C2B-C3B-CAB-CBB
24	6	613	CLA	C2B-C3B-CAB-CBB
24	6	614	CLA	C2B-C3B-CAB-CBB
24	8	302	CLA	C2B-C3B-CAB-CBB
24	8	303	CLA	C2B-C3B-CAB-CBB
24	B	605	CLA	C2B-C3B-CAB-CBB
24	B	615	CLA	C2B-C3B-CAB-CBB
24	G	610	CLA	C2B-C3B-CAB-CBB
24	N	602	CLA	C2B-C3B-CAB-CBB
24	S	611	CLA	C2B-C3B-CAB-CBB
24	S	613	CLA	C2B-C3B-CAB-CBB
24	Y	312	CLA	C2B-C3B-CAB-CBB
24	b	616	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	d	402	CLA	C2B-C3B-CAB-CBB
24	g	603	CLA	C2B-C3B-CAB-CBB
24	n	611	CLA	C2B-C3B-CAB-CBB
24	n	613	CLA	C2B-C3B-CAB-CBB
24	A	405	CLA	C2B-C3B-CAB-CBB
24	A	407	CLA	C2B-C3B-CAB-CBB
24	a	405	CLA	C2B-C3B-CAB-CBB
24	a	407	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C2B-C3B-CAB-CBB
24	r	601	CLA	C2B-C3B-CAB-CBB
24	9	611	CLA	C2B-C3B-CAB-CBB
24	9	612	CLA	C2B-C3B-CAB-CBB
24	0	614	CLA	C2B-C3B-CAB-CBB
24	AA	304	CLA	C2B-C3B-CAB-CBB
24	AB	302	CLA	C2B-C3B-CAB-CBB
24	AB	303	CLA	C2B-C3B-CAB-CBB
24	v	605	CLA	C2B-C3B-CAB-CBB
24	Au	610	CLA	C2B-C3B-CAB-CBB
24	Au	612	CLA	C2B-C3B-CAB-CBB
24	A6	613	CLA	C2B-C3B-CAB-CBB
24	BE	616	CLA	C2B-C3B-CAB-CBB
24	BQ	611	CLA	C2B-C3B-CAB-CBB
24	BQ	613	CLA	C2B-C3B-CAB-CBB
24	BV	603	CLA	C2B-C3B-CAB-CBB
24	R	404	CLA	C2B-C3B-CAB-CBB
24	R	406	CLA	C2B-C3B-CAB-CBB
24	BD	407	CLA	C2B-C3B-CAB-CBB
24	BF	514	CLA	C2B-C3B-CAB-CBB
24	BU	608	CLA	C2B-C3B-CAB-CBB
23	AA	310	CHL	C4C-C3C-CAC-CBC
29	b	619	BCR	C16-C17-C18-C36
24	c	511	CLA	C4-C3-C5-C6
23	A2	605	CHL	CAA-CBA-CGA-O2A
23	A2	606	CHL	CAA-CBA-CGA-O2A
32	R	411	SQD	O47-C7-C8-C9
27	v	621	LHG	C12-C13-C14-C15
24	BF	503	CLA	O1A-CGA-O2A-C1
23	n	607	CHL	C2-C3-C5-C6
23	BQ	607	CHL	C2-C3-C5-C6
24	a	405	CLA	C15-C16-C17-C18
24	9	602	CLA	C8-C10-C11-C12
24	v	601	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	BJ	603	CLA	C5-C6-C7-C8
24	v	601	CLA	C16-C17-C18-C19
27	C	520	LHG	C32-C33-C34-C35
27	1	520	LHG	C32-C33-C34-C35
27	BF	520	LHG	C29-C30-C31-C32
31	D	403	PL9	C47-C48-C49-C51
30	B	620	LMG	C37-C38-C39-C40
24	B	601	CLA	C13-C15-C16-C17
24	g	603	CLA	C5-C6-C7-C8
24	v	616	CLA	C13-C15-C16-C17
24	BD	405	CLA	C15-C16-C17-C18
23	G	606	CHL	C1-C2-C3-C4
23	N	606	CHL	C1-C2-C3-C4
23	Y	307	CHL	C1-C2-C3-C4
23	g	606	CHL	C1-C2-C3-C4
23	n	606	CHL	C1-C2-C3-C4
23	y	307	CHL	C1-C2-C3-C4
23	Au	606	CHL	C1-C2-C3-C4
23	A2	606	CHL	C1-C2-C3-C4
23	BB	307	CHL	C1-C2-C3-C4
23	BJ	606	CHL	C1-C2-C3-C4
23	BQ	606	CHL	C1-C2-C3-C4
23	Ba	307	CHL	C1-C2-C3-C4
24	S	611	CLA	C1-C2-C3-C4
24	S	613	CLA	C1-C2-C3-C4
24	s	611	CLA	C1-C2-C3-C4
24	s	613	CLA	C1-C2-C3-C4
24	r	601	CLA	C1-C2-C3-C4
24	r	611	CLA	C1-C2-C3-C4
24	A6	611	CLA	C1-C2-C3-C4
24	A6	613	CLA	C1-C2-C3-C4
24	BV	611	CLA	C1-C2-C3-C4
24	BV	613	CLA	C1-C2-C3-C4
24	BU	601	CLA	C1-C2-C3-C4
24	BU	611	CLA	C1-C2-C3-C4
24	0	602	CLA	O1D-CGD-O2D-CED
24	v	604	CLA	C3-C5-C6-C7
23	Y	308	CHL	O1D-CGD-O2D-CED
24	r	604	CLA	O1D-CGD-O2D-CED
23	N	606	CHL	CAA-CBA-CGA-O2A
24	BG	401	CLA	CAA-CBA-CGA-O2A
27	BE	623	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	c	519	LHG	C6-C5-O7-C7
23	A2	609	CHL	C2A-CAA-CBA-CGA
24	g	610	CLA	C2A-CAA-CBA-CGA
24	n	602	CLA	C2A-CAA-CBA-CGA
24	AA	304	CLA	C2A-CAA-CBA-CGA
24	BJ	610	CLA	C2A-CAA-CBA-CGA
30	BE	621	LMG	C37-C38-C39-C40
24	B	606	CLA	C2-C1-O2A-CGA
24	B	615	CLA	C2-C1-O2A-CGA
24	Y	311	CLA	C2-C1-O2A-CGA
24	d	401	CLA	C2-C1-O2A-CGA
24	a	407	CLA	C2-C1-O2A-CGA
24	r	601	CLA	C2-C1-O2A-CGA
24	r	604	CLA	C2-C1-O2A-CGA
24	0	610	CLA	C2-C1-O2A-CGA
24	AA	303	CLA	C2-C1-O2A-CGA
24	v	606	CLA	C2-C1-O2A-CGA
24	v	615	CLA	C2-C1-O2A-CGA
24	BB	311	CLA	C2-C1-O2A-CGA
24	BG	401	CLA	C2-C1-O2A-CGA
24	Ba	311	CLA	C2-C1-O2A-CGA
24	1	512	CLA	C2-C1-O2A-CGA
24	BD	407	CLA	C2-C1-O2A-CGA
24	BU	601	CLA	C2-C1-O2A-CGA
23	BU	607	CHL	C2C-C3C-CAC-CBC
30	BF	519	LMG	C39-C40-C41-C42
27	Ba	319	LHG	C23-C24-C25-C26
30	c	518	LMG	C39-C40-C41-C42
32	D	406	SQD	C12-C13-C14-C15
23	N	605	CHL	CAA-CBA-CGA-O2A
23	n	606	CHL	CAA-CBA-CGA-O2A
23	BQ	606	CHL	CAA-CBA-CGA-O2A
24	B	601	CLA	CAA-CBA-CGA-O2A
24	2	402	CLA	CAA-CBA-CGA-O2A
24	BE	602	CLA	CAA-CBA-CGA-O2A
32	A	413	SQD	O47-C7-C8-C9
23	n	609	CHL	C13-C15-C16-C17
24	C	505	CLA	C5-C6-C7-C8
24	B	604	CLA	C3-C5-C6-C7
24	c	512	CLA	C3-C5-C6-C7
24	2	402	CLA	C3-C5-C6-C7
27	A2	618	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
27	1	520	LHG	C9-C10-C11-C12
24	1	507	CLA	C8-C10-C11-C12
27	Y	319	LHG	C11-C12-C13-C14
27	y	319	LHG	C10-C11-C12-C13
27	2	405	LHG	C24-C25-C26-C27
24	n	602	CLA	O1A-CGA-O2A-C1
27	g	618	LHG	C29-C30-C31-C32
27	v	621	LHG	C29-C30-C31-C32
27	BE	623	LHG	C33-C34-C35-C36
30	1	501	LMG	C12-C13-C14-C15
24	b	602	CLA	CAA-CBA-CGA-O2A
24	b	603	CLA	CAA-CBA-CGA-O2A
24	BE	610	CLA	C4-C3-C5-C6
23	BB	308	CHL	O1D-CGD-O2D-CED
29	8	313	BCR	C23-C24-C25-C30
29	B	619	BCR	C23-C24-C25-C26
29	b	601	BCR	C23-C24-C25-C26
29	b	619	BCR	C1-C6-C7-C8
29	b	619	BCR	C23-C24-C25-C30
29	C	515	BCR	C5-C6-C7-C8
29	a	411	BCR	C5-C6-C7-C8
29	c	515	BCR	C1-C6-C7-C8
29	BE	601	BCR	C23-C24-C25-C26
29	BE	619	BCR	C1-C6-C7-C8
29	BE	619	BCR	C23-C24-C25-C30
29	1	515	BCR	C5-C6-C7-C8
29	BF	516	BCR	C1-C6-C7-C8
24	b	608	CLA	C2-C3-C5-C6
30	1	519	LMG	C39-C40-C41-C42
34	R	401	DGD	C6B-C7B-C8B-C9B
24	n	602	CLA	CBA-CGA-O2A-C1
30	d	405	LMG	C29-C28-O8-C9
30	BG	405	LMG	C29-C28-O8-C9
24	D	401	CLA	CAA-CBA-CGA-O2A
24	v	601	CLA	CAA-CBA-CGA-O2A
27	BB	319	LHG	C11-C12-C13-C14
24	v	611	CLA	C5-C6-C7-C8
24	0	613	CLA	O1A-CGA-O2A-C1
23	7	308	CHL	C11-C12-C13-C15
24	BV	612	CLA	C6-C7-C8-C9
24	BF	503	CLA	C16-C17-C18-C19
34	1	516	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
32	l	102	SQD	C7-C8-C9-C10
24	C	507	CLA	C8-C10-C11-C12
23	BB	306	CHL	C2A-CAA-CBA-CGA
24	7	304	CLA	C2A-CAA-CBA-CGA
24	1	507	CLA	C2A-CAA-CBA-CGA
26	g	617	NEX	C28-C29-C30-C31
26	9	617	NEX	C28-C29-C30-C31
26	A6	616	NEX	C28-C29-C30-C31
26	BJ	617	NEX	C28-C29-C30-C31
34	a	413	DGD	C2D-C1D-O3G-C3G
34	BD	413	DGD	C2D-C1D-O3G-C3G
27	y	319	LHG	C30-C31-C32-C33
27	y	319	LHG	O7-C5-C6-O8
27	Ba	319	LHG	O7-C5-C6-O8
30	A	412	LMG	O1-C7-C8-O7
30	A	412	LMG	O7-C8-C9-O8
30	BL	101	LMG	O1-C7-C8-O7
23	6	607	CHL	C4C-C3C-CAC-CBC
30	C	501	LMG	C12-C13-C14-C15
30	C	519	LMG	C39-C40-C41-C42
32	2	408	SQD	C12-C13-C14-C15
30	v	623	LMG	C29-C28-O8-C9
27	B	621	LHG	C3-O3-P-O6
27	D	404	LHG	C3-O3-P-O6
27	b	622	LHG	C3-O3-P-O6
27	b	624	LHG	C3-O3-P-O6
27	d	404	LHG	C3-O3-P-O6
27	C	520	LHG	C4-O6-P-O3
27	c	519	LHG	C4-O6-P-O3
27	v	621	LHG	C3-O3-P-O6
27	2	406	LHG	C3-O3-P-O6
27	BE	622	LHG	C3-O3-P-O6
27	BG	404	LHG	C3-O3-P-O6
27	1	520	LHG	C4-O6-P-O3
27	BF	520	LHG	C4-O6-P-O3
27	y	319	LHG	C23-C24-C25-C26
27	B	621	LHG	C12-C13-C14-C15
27	BB	319	LHG	C28-C29-C30-C31
24	c	503	CLA	C16-C17-C18-C19
38	a	409	PHO	CHA-CBD-CGD-O1D
34	A	402	DGD	C6B-C7B-C8B-C9B
24	BE	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	6	603	CLA	C5-C6-C7-C8
24	b	603	CLA	C8-C10-C11-C12
27	y	319	LHG	C25-C26-C27-C28
27	g	618	LHG	C4-C5-C6-O8
27	BJ	618	LHG	C4-C5-C6-O8
30	BG	405	LMG	O1-C7-C8-C9
34	C	517	DGD	C1G-C2G-C3G-O3G
34	a	413	DGD	C1G-C2G-C3G-O3G
34	1	517	DGD	C1G-C2G-C3G-O3G
34	BD	413	DGD	C1G-C2G-C3G-O3G
24	C	510	CLA	C4-C3-C5-C6
24	BF	511	CLA	C4-C3-C5-C6
27	BJ	618	LHG	C29-C30-C31-C32
34	a	401	DGD	C4A-C5A-C6A-C7A
34	1	518	DGD	C4E-C5E-C6E-O5E
23	G	607	CHL	C11-C12-C13-C15
23	n	607	CHL	C11-C12-C13-C15
23	y	308	CHL	C11-C12-C13-C15
23	Au	607	CHL	C11-C12-C13-C15
23	BQ	607	CHL	C11-C12-C13-C15
24	B	607	CLA	C11-C10-C8-C7
24	c	507	CLA	C11-C12-C13-C15
24	v	615	CLA	C11-C10-C8-C7
24	BB	313	CLA	C2-C3-C5-C6
24	BQ	612	CLA	C6-C7-C8-C10
27	BE	622	LHG	C26-C27-C28-C29
34	a	401	DGD	C2B-C3B-C4B-C5B
34	C	518	DGD	C4E-C5E-C6E-O5E
23	G	601	CHL	C11-C12-C13-C14
23	G	607	CHL	C14-C13-C15-C16
23	N	601	CHL	C11-C12-C13-C14
23	y	309	CHL	C11-C12-C13-C14
23	y	310	CHL	C11-C12-C13-C14
23	Au	601	CHL	C11-C12-C13-C14
23	Au	607	CHL	C14-C13-C15-C16
23	A2	601	CHL	C11-C12-C13-C14
23	BJ	607	CHL	C14-C13-C15-C16
23	Ba	309	CHL	C11-C12-C13-C14
24	B	606	CLA	C14-C13-C15-C16
24	B	616	CLA	C6-C7-C8-C9
24	Y	314	CLA	C11-C12-C13-C14
24	b	608	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	613	CLA	C11-C10-C8-C9
24	b	617	CLA	C6-C7-C8-C9
24	g	610	CLA	C11-C10-C8-C9
24	g	613	CLA	C6-C7-C8-C9
24	n	602	CLA	C6-C7-C8-C9
24	C	509	CLA	C11-C10-C8-C9
24	C	510	CLA	C14-C13-C15-C16
24	c	510	CLA	C11-C10-C8-C9
24	r	602	CLA	C6-C7-C8-C9
24	v	606	CLA	C14-C13-C15-C16
24	Au	610	CLA	C11-C12-C13-C14
24	BB	314	CLA	C11-C12-C13-C14
24	BE	608	CLA	C11-C10-C8-C9
24	BE	613	CLA	C11-C10-C8-C9
24	BE	617	CLA	C6-C7-C8-C9
24	BJ	610	CLA	C11-C10-C8-C9
24	BJ	613	CLA	C6-C7-C8-C9
24	1	509	CLA	C11-C10-C8-C9
24	BF	510	CLA	C11-C10-C8-C9
24	BU	602	CLA	C6-C7-C8-C9
23	Au	607	CHL	C15-C16-C17-C18
28	N	619	XAT	C13-C14-C15-C35
28	AA	301	XAT	C13-C14-C15-C35
29	B	623	BCR	C19-C20-C21-C22
23	n	608	CHL	C16-C17-C18-C20
38	A	409	PHO	C16-C17-C18-C20
32	BO	102	SQD	C7-C8-C9-C10
27	b	622	LHG	C26-C27-C28-C29
27	A2	618	LHG	C9-C10-C11-C12
30	BE	621	LMG	C29-C30-C31-C32
32	BO	101	SQD	C29-C30-C31-C32
30	B	624	LMG	C29-C28-O8-C9
27	BE	622	LHG	C31-C32-C33-C34
32	a	412	SQD	C15-C16-C17-C18
23	BJ	608	CHL	CAA-CBA-CGA-O2A
24	6	613	CLA	C5-C6-C7-C8
27	b	622	LHG	C31-C32-C33-C34
27	Ba	319	LHG	C10-C11-C12-C13
30	b	621	LMG	C40-C41-C42-C43
25	6	615	LUT	C7-C8-C9-C19
27	N	618	LHG	C9-C10-C11-C12
27	c	519	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	y	319	LHG	C2-C3-O3-P
27	Ba	319	LHG	C2-C3-O3-P
27	n	618	LHG	C27-C28-C29-C30
23	g	608	CHL	CAA-CBA-CGA-O2A
24	B	608	CLA	C13-C15-C16-C17
25	A6	614	LUT	C7-C8-C9-C10
28	BB	301	XAT	C7-C8-C9-C10
27	BQ	618	LHG	C27-C28-C29-C30
27	BF	520	LHG	C9-C10-C11-C12
24	1	503	CLA	C3-C5-C6-C7
24	S	602	CLA	C12-C13-C15-C16
24	A6	602	CLA	C12-C13-C15-C16
27	b	623	LHG	C29-C30-C31-C32
27	r	618	LHG	C15-C16-C17-C18
24	1	510	CLA	C4-C3-C5-C6
27	1	520	LHG	C7-C8-C9-C10
24	Y	313	CLA	C2-C3-C5-C6
24	BV	609	CLA	C2-C3-C5-C6
23	AA	308	CHL	C11-C12-C13-C15
24	s	612	CLA	C6-C7-C8-C9
23	7	308	CHL	CBA-CGA-O2A-C1
23	r	605	CHL	CBA-CGA-O2A-C1
24	BB	303	CLA	CBA-CGA-O2A-C1
27	BF	521	LHG	C24-C23-O8-C6
34	c	517	DGD	CBB-CCB-CDB-CEB
24	b	612	CLA	C10-C11-C12-C13
23	5	601	CHL	CAA-CBA-CGA-O2A
23	9	601	CHL	CAA-CBA-CGA-O2A
30	BE	621	LMG	C40-C41-C42-C43
32	l	101	SQD	C29-C30-C31-C32
32	BD	412	SQD	C15-C16-C17-C18
24	Y	304	CLA	C5-C6-C7-C8
23	r	605	CHL	O1A-CGA-O2A-C1
27	Ba	319	LHG	O10-C23-O8-C6
24	6	613	CLA	CBA-CGA-O2A-C1
27	c	520	LHG	C24-C23-O8-C6
32	D	406	SQD	C24-C23-O48-C46
27	BU	617	LHG	C27-C28-C29-C30
34	BD	401	DGD	C4A-C5A-C6A-C7A
23	S	605	CHL	C4B-C3B-CAB-CBB
23	AA	309	CHL	C4B-C3B-CAB-CBB
23	A6	605	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	6	602	CLA	C4B-C3B-CAB-CBB
24	B	605	CLA	C4B-C3B-CAB-CBB
24	D	402	CLA	C4B-C3B-CAB-CBB
24	N	602	CLA	C4B-C3B-CAB-CBB
24	S	613	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
24	s	603	CLA	C4B-C3B-CAB-CBB
24	A	405	CLA	C4B-C3B-CAB-CBB
24	a	405	CLA	C4B-C3B-CAB-CBB
24	v	605	CLA	C4B-C3B-CAB-CBB
24	Au	610	CLA	C4B-C3B-CAB-CBB
24	A6	613	CLA	C4B-C3B-CAB-CBB
24	BE	606	CLA	C4B-C3B-CAB-CBB
24	BG	402	CLA	C4B-C3B-CAB-CBB
24	BJ	603	CLA	C4B-C3B-CAB-CBB
24	BV	603	CLA	C4B-C3B-CAB-CBB
24	Ba	311	CLA	C4B-C3B-CAB-CBB
24	R	404	CLA	C4B-C3B-CAB-CBB
24	1	505	CLA	C4B-C3B-CAB-CBB
24	1	513	CLA	C4B-C3B-CAB-CBB
24	BF	514	CLA	C4B-C3B-CAB-CBB
23	6	607	CHL	C2A-CAA-CBA-CGA
24	BQ	602	CLA	C2A-CAA-CBA-CGA
24	BU	604	CLA	C2A-CAA-CBA-CGA
26	BQ	617	NEX	C33-C34-C35-C15
26	BV	616	NEX	C29-C30-C31-C32
28	7	301	XAT	C13-C14-C15-C35
28	A2	619	XAT	C13-C14-C15-C35
29	BE	601	BCR	C19-C20-C21-C22
27	BU	617	LHG	C15-C16-C17-C18
34	BD	401	DGD	C2B-C3B-C4B-C5B
27	b	624	LHG	O10-C23-O8-C6
34	BK	102	DGD	O1A-C1A-O1G-C1G
27	b	622	LHG	C12-C13-C14-C15
27	G	618	LHG	C17-C18-C19-C20
27	BE	622	LHG	C12-C13-C14-C15
23	g	601	CHL	C16-C17-C18-C19
24	9	613	CLA	C4-C3-C5-C6
24	v	609	CLA	C4-C3-C5-C6
24	1	504	CLA	C13-C15-C16-C17
34	a	413	DGD	C4D-C5D-C6D-O5D
34	BD	413	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
24	9	613	CLA	C2-C3-C5-C6
31	BG	403	PL9	C43-C44-C46-C47
23	7	308	CHL	O1A-CGA-O2A-C1
27	y	319	LHG	O10-C23-O8-C6
27	0	617	LHG	O10-C23-O8-C6
32	D	406	SQD	O10-C23-O48-C46
27	Au	618	LHG	C17-C18-C19-C20
27	Ba	319	LHG	C25-C26-C27-C28
27	BU	617	LHG	C14-C15-C16-C17
30	BF	501	LMG	C38-C39-C40-C41
24	B	610	CLA	C2-C1-O2A-CGA
24	B	616	CLA	C2-C1-O2A-CGA
24	b	607	CLA	C2-C1-O2A-CGA
24	b	611	CLA	C2-C1-O2A-CGA
24	n	604	CLA	C2-C1-O2A-CGA
24	y	304	CLA	C2-C1-O2A-CGA
24	A	410	CLA	C2-C1-O2A-CGA
24	C	512	CLA	C2-C1-O2A-CGA
24	a	410	CLA	C2-C1-O2A-CGA
24	v	610	CLA	C2-C1-O2A-CGA
24	v	616	CLA	C2-C1-O2A-CGA
24	BE	607	CLA	C2-C1-O2A-CGA
24	BE	611	CLA	C2-C1-O2A-CGA
24	BE	617	CLA	C2-C1-O2A-CGA
24	BQ	604	CLA	C2-C1-O2A-CGA
24	Ba	304	CLA	C2-C1-O2A-CGA
24	BD	410	CLA	C2-C1-O2A-CGA
24	BU	604	CLA	C2-C1-O2A-CGA
24	5	602	CLA	C2C-C3C-CAC-CBC
27	2	406	LHG	C32-C33-C34-C35
23	BQ	608	CHL	C16-C17-C18-C20
24	A2	611	CLA	C11-C12-C13-C14
27	BF	521	LHG	C25-C26-C27-C28
27	Au	618	LHG	C29-C30-C31-C32
23	Y	306	CHL	C2A-CAA-CBA-CGA
23	0	607	CHL	C2A-CAA-CBA-CGA
24	7	311	CLA	C2A-CAA-CBA-CGA
24	C	510	CLA	C2A-CAA-CBA-CGA
24	AA	311	CLA	C2A-CAA-CBA-CGA
24	1	510	CLA	C2A-CAA-CBA-CGA
27	g	618	LHG	O7-C5-C6-O8
27	BJ	618	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	O2G-C2G-C3G-O3G
34	1	517	DGD	O2G-C2G-C3G-O3G
34	1	517	DGD	C5A-C6A-C7A-C8A
24	B	602	CLA	CAA-CBA-CGA-O2A
24	n	602	CLA	C15-C16-C17-C18
27	6	617	LHG	C2-C3-O3-P
23	7	307	CHL	C3A-C2A-CAA-CBA
23	8	305	CHL	C3A-C2A-CAA-CBA
23	G	601	CHL	C3A-C2A-CAA-CBA
23	Y	302	CHL	C3A-C2A-CAA-CBA
23	AA	307	CHL	C3A-C2A-CAA-CBA
23	Au	601	CHL	C3A-C2A-CAA-CBA
23	BQ	606	CHL	C3A-C2A-CAA-CBA
23	Ba	302	CHL	C3A-C2A-CAA-CBA
24	B	601	CLA	C3A-C2A-CAA-CBA
24	y	314	CLA	C3A-C2A-CAA-CBA
24	v	601	CLA	C3A-C2A-CAA-CBA
24	BQ	604	CLA	C3A-C2A-CAA-CBA
24	Ba	314	CLA	C3A-C2A-CAA-CBA
23	5	601	CHL	CAA-CBA-CGA-O1A
23	9	601	CHL	CAA-CBA-CGA-O1A
24	BU	614	CLA	CAA-CBA-CGA-O2A
30	b	621	LMG	C29-C30-C31-C32
23	G	607	CHL	C15-C16-C17-C18
24	7	303	CLA	C2C-C3C-CAC-CBC
23	A6	605	CHL	CAA-CBA-CGA-O1A
24	r	614	CLA	CAA-CBA-CGA-O2A
24	5	613	CLA	C4-C3-C5-C6
31	D	403	PL9	C45-C44-C46-C47
27	BB	319	LHG	C29-C30-C31-C32
27	G	618	LHG	C29-C30-C31-C32
23	Y	310	CHL	C11-C12-C13-C14
23	BB	310	CHL	C11-C12-C13-C14
24	B	601	CLA	C14-C13-C15-C16
24	B	604	CLA	C14-C13-C15-C16
24	B	608	CLA	C11-C10-C8-C9
24	G	602	CLA	C14-C13-C15-C16
24	G	612	CLA	C6-C7-C8-C9
24	N	603	CLA	C6-C7-C8-C9
24	Y	312	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C10-C8-C9
24	g	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	g	610	CLA	C6-C7-C8-C9
24	c	513	CLA	C11-C10-C8-C9
24	v	601	CLA	C14-C13-C15-C16
24	v	604	CLA	C14-C13-C15-C16
24	v	608	CLA	C11-C10-C8-C9
24	v	616	CLA	C6-C7-C8-C9
24	v	616	CLA	C11-C10-C8-C9
24	Au	612	CLA	C6-C7-C8-C9
24	A2	603	CLA	C6-C7-C8-C9
24	BE	609	CLA	C11-C12-C13-C14
24	BE	614	CLA	C11-C10-C8-C9
24	BJ	602	CLA	C11-C10-C8-C9
24	BJ	603	CLA	C6-C7-C8-C9
24	BJ	610	CLA	C6-C7-C8-C9
24	Ba	312	CLA	C6-C7-C8-C9
24	BF	513	CLA	C11-C10-C8-C9
38	R	408	PHO	C16-C17-C18-C20
27	W	201	LHG	C15-C16-C17-C18
27	BJ	618	LHG	C9-C10-C11-C12
24	BU	614	CLA	CAA-CBA-CGA-O1A
24	B	611	CLA	C5-C6-C7-C8
24	N	603	CLA	C5-C6-C7-C8
24	b	606	CLA	C10-C11-C12-C13
24	0	603	CLA	C5-C6-C7-C8
24	v	608	CLA	C13-C15-C16-C17
24	BB	304	CLA	C5-C6-C7-C8
24	BE	606	CLA	C10-C11-C12-C13
24	R	404	CLA	C15-C16-C17-C18
27	C	520	LHG	C7-C8-C9-C10
27	g	618	LHG	C9-C10-C11-C12
34	BD	401	DGD	C8B-C9B-CAB-CBB
24	BG	402	CLA	O1D-CGD-O2D-CED
23	0	607	CHL	C3-C5-C6-C7
27	G	618	LHG	C30-C31-C32-C33
27	0	617	LHG	C35-C36-C37-C38
27	A0	202	LHG	C15-C16-C17-C18
27	BY	201	LHG	C31-C32-C33-C34
26	Y	318	NEX	C39-C29-C30-C31
26	g	617	NEX	C39-C29-C30-C31
26	n	617	NEX	C39-C29-C30-C31
26	9	617	NEX	C39-C29-C30-C31
26	A2	617	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	A6	616	NEX	C39-C29-C30-C31
26	BB	318	NEX	C39-C29-C30-C31
26	BJ	617	NEX	C39-C29-C30-C31
27	Y	319	LHG	C4-C5-C6-O8
27	Az	102	LHG	C1-C2-C3-O3
29	B	623	BCR	C16-C17-C18-C36
29	v	619	BCR	C11-C10-C9-C34
29	Bb	101	BCR	C20-C21-C22-C37
30	B	620	LMG	O9-C10-O7-C8
24	AA	314	CLA	CAA-CBA-CGA-O2A
24	6	602	CLA	O1D-CGD-O2D-CED
23	g	605	CHL	C2A-CAA-CBA-CGA
23	BJ	605	CHL	C2A-CAA-CBA-CGA
24	BG	401	CLA	C2A-CAA-CBA-CGA
24	b	617	CLA	C13-C15-C16-C17
34	C	517	DGD	C5A-C6A-C7A-C8A
23	S	606	CHL	O2A-C1-C2-C3
23	s	606	CHL	O2A-C1-C2-C3
23	A6	606	CHL	O2A-C1-C2-C3
23	BV	606	CHL	O2A-C1-C2-C3
23	BU	605	CHL	CBA-CGA-O2A-C1
24	0	613	CLA	CBA-CGA-O2A-C1
27	b	623	LHG	C24-C23-O8-C6
30	BF	519	LMG	C40-C41-C42-C43
23	AA	302	CHL	CAA-CBA-CGA-O1A
24	7	314	CLA	CAA-CBA-CGA-O2A
24	r	614	CLA	CAA-CBA-CGA-O1A
26	G	617	NEX	C31-C32-C33-C40
29	B	617	BCR	C37-C22-C23-C24
29	v	617	BCR	C37-C22-C23-C24
23	BU	605	CHL	O1A-CGA-O2A-C1
27	1	520	LHG	C24-C25-C26-C27
24	B	616	CLA	C13-C15-C16-C17
24	BE	605	CLA	C10-C11-C12-C13
24	BQ	602	CLA	C15-C16-C17-C18
34	a	401	DGD	C8B-C9B-CAB-CBB
25	S	614	LUT	C7-C8-C9-C10
28	Y	301	XAT	C7-C8-C9-C10
27	w	201	LHG	C31-C32-C33-C34
27	r	618	LHG	C14-C15-C16-C17
23	A6	605	CHL	CAA-CBA-CGA-O2A
31	2	404	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
23	6	601	CHL	C1A-C2A-CAA-CBA
23	6	608	CHL	C1A-C2A-CAA-CBA
23	7	302	CHL	C1A-C2A-CAA-CBA
23	G	601	CHL	C1A-C2A-CAA-CBA
23	G	606	CHL	C1A-C2A-CAA-CBA
23	G	609	CHL	C1A-C2A-CAA-CBA
23	Y	302	CHL	C1A-C2A-CAA-CBA
23	g	601	CHL	C1A-C2A-CAA-CBA
23	n	601	CHL	C1A-C2A-CAA-CBA
23	n	609	CHL	C1A-C2A-CAA-CBA
23	y	310	CHL	C1A-C2A-CAA-CBA
23	0	601	CHL	C1A-C2A-CAA-CBA
23	0	608	CHL	C1A-C2A-CAA-CBA
23	AA	302	CHL	C1A-C2A-CAA-CBA
23	Au	606	CHL	C1A-C2A-CAA-CBA
23	Au	609	CHL	C1A-C2A-CAA-CBA
23	BB	302	CHL	C1A-C2A-CAA-CBA
23	BJ	601	CHL	C1A-C2A-CAA-CBA
23	BQ	601	CHL	C1A-C2A-CAA-CBA
23	BQ	609	CHL	C1A-C2A-CAA-CBA
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	C1A-C2A-CAA-CBA
24	n	604	CLA	C1A-C2A-CAA-CBA
24	y	314	CLA	C1A-C2A-CAA-CBA
24	c	504	CLA	C1A-C2A-CAA-CBA
24	c	507	CLA	C1A-C2A-CAA-CBA
24	v	601	CLA	C1A-C2A-CAA-CBA
24	v	602	CLA	C1A-C2A-CAA-CBA
24	BB	303	CLA	C1A-C2A-CAA-CBA
24	BQ	604	CLA	C1A-C2A-CAA-CBA
24	Ba	314	CLA	C1A-C2A-CAA-CBA
24	BF	507	CLA	C1A-C2A-CAA-CBA
24	d	401	CLA	CAA-CBA-CGA-O2A
23	N	607	CHL	C2-C3-C5-C6
23	g	608	CHL	C11-C12-C13-C15
23	BJ	608	CHL	C11-C12-C13-C15
23	Ba	308	CHL	C11-C12-C13-C15
24	5	613	CLA	C2-C3-C5-C6
24	D	402	CLA	C11-C12-C13-C15
24	G	610	CLA	C11-C10-C8-C7
24	I	102	CLA	C12-C13-C15-C16
24	N	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	Y	304	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	n	612	CLA	C6-C7-C8-C10
24	C	510	CLA	C11-C10-C8-C7
24	2	403	CLA	C11-C12-C13-C15
24	BE	616	CLA	C11-C10-C8-C7
24	1	510	CLA	C11-C10-C8-C7
24	Y	312	CLA	C8-C10-C11-C12
24	b	602	CLA	C13-C15-C16-C17
24	b	612	CLA	C5-C6-C7-C8
24	A	405	CLA	C15-C16-C17-C18
23	S	605	CHL	CAA-CBA-CGA-O1A
24	7	314	CLA	CAA-CBA-CGA-O1A
24	AA	314	CLA	CAA-CBA-CGA-O1A
30	c	501	LMG	C38-C39-C40-C41
26	s	616	NEX	C29-C30-C31-C32
23	8	306	CHL	C3C-C2C-CMC-OMC
23	G	606	CHL	C3C-C2C-CMC-OMC
23	g	609	CHL	C3C-C2C-CMC-OMC
23	r	613	CHL	C3C-C2C-CMC-OMC
23	AB	307	CHL	C3C-C2C-CMC-OMC
23	Au	606	CHL	C3C-C2C-CMC-OMC
23	BJ	609	CHL	C3C-C2C-CMC-OMC
27	c	519	LHG	C30-C31-C32-C33
24	v	602	CLA	CAA-CBA-CGA-O2A
23	7	302	CHL	CAA-CBA-CGA-O1A
24	b	605	CLA	C10-C11-C12-C13
27	b	624	LHG	C13-C14-C15-C16
27	w	201	LHG	C15-C16-C17-C18
27	r	618	LHG	C27-C28-C29-C30
27	0	617	LHG	C2-C3-O3-P
24	7	305	CLA	C2A-CAA-CBA-CGA
24	B	605	CLA	C2A-CAA-CBA-CGA
24	G	610	CLA	C2A-CAA-CBA-CGA
24	AA	305	CLA	C2A-CAA-CBA-CGA
24	v	605	CLA	C2A-CAA-CBA-CGA
24	Au	610	CLA	C2A-CAA-CBA-CGA
24	S	602	CLA	C5-C6-C7-C8
24	v	605	CLA	C13-C15-C16-C17
24	BE	610	CLA	C13-C15-C16-C17
24	BE	614	CLA	C5-C6-C7-C8
24	BE	617	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	BF	520	LHG	C16-C17-C18-C19
24	BB	303	CLA	O1A-CGA-O2A-C1
23	6	605	CHL	O1D-CGD-O2D-CED
24	AA	312	CLA	CAA-CBA-CGA-O2A
27	g	618	LHG	C31-C32-C33-C34
27	BE	624	LHG	C13-C14-C15-C16
27	BB	319	LHG	O6-C4-C5-C6
30	b	621	LMG	O6-C5-C6-O5
23	S	605	CHL	CAA-CBA-CGA-O2A
23	AA	307	CHL	CAA-CBA-CGA-O2A
27	BY	201	LHG	C15-C16-C17-C18
34	H	102	DGD	O2G-C1B-C2B-C3B
34	Av	102	DGD	O2G-C1B-C2B-C3B
31	d	403	PL9	C20-C19-C21-C22
27	n	618	LHG	C34-C35-C36-C37
30	c	518	LMG	C40-C41-C42-C43
24	r	602	CLA	C8-C10-C11-C12
23	5	605	CHL	C2B-C3B-CAB-CBB
23	7	309	CHL	C2B-C3B-CAB-CBB
23	8	305	CHL	C2B-C3B-CAB-CBB
23	S	605	CHL	C2B-C3B-CAB-CBB
23	S	607	CHL	C2B-C3B-CAB-CBB
23	9	605	CHL	C2B-C3B-CAB-CBB
23	AA	309	CHL	C2B-C3B-CAB-CBB
23	AB	305	CHL	C2B-C3B-CAB-CBB
23	A6	605	CHL	C2B-C3B-CAB-CBB
23	A6	607	CHL	C2B-C3B-CAB-CBB
24	5	603	CLA	C2B-C3B-CAB-CBB
24	5	612	CLA	C2B-C3B-CAB-CBB
24	7	304	CLA	C2B-C3B-CAB-CBB
24	8	309	CLA	C2B-C3B-CAB-CBB
24	G	603	CLA	C2B-C3B-CAB-CBB
24	G	612	CLA	C2B-C3B-CAB-CBB
24	N	613	CLA	C2B-C3B-CAB-CBB
24	S	608	CLA	C2B-C3B-CAB-CBB
24	Y	304	CLA	C2B-C3B-CAB-CBB
24	Y	313	CLA	C2B-C3B-CAB-CBB
24	g	611	CLA	C2B-C3B-CAB-CBB
24	n	603	CLA	C2B-C3B-CAB-CBB
24	s	603	CLA	C2B-C3B-CAB-CBB
24	s	610	CLA	C2B-C3B-CAB-CBB
24	y	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	y	312	CLA	C2B-C3B-CAB-CBB
24	c	504	CLA	C2B-C3B-CAB-CBB
24	c	513	CLA	C2B-C3B-CAB-CBB
24	c	514	CLA	C2B-C3B-CAB-CBB
24	r	614	CLA	C2B-C3B-CAB-CBB
24	AB	309	CLA	C2B-C3B-CAB-CBB
24	Au	603	CLA	C2B-C3B-CAB-CBB
24	A2	602	CLA	C2B-C3B-CAB-CBB
24	A6	608	CLA	C2B-C3B-CAB-CBB
24	BB	304	CLA	C2B-C3B-CAB-CBB
24	BB	312	CLA	C2B-C3B-CAB-CBB
24	BB	313	CLA	C2B-C3B-CAB-CBB
24	BG	402	CLA	C2B-C3B-CAB-CBB
24	BJ	603	CLA	C2B-C3B-CAB-CBB
24	BJ	611	CLA	C2B-C3B-CAB-CBB
24	BQ	603	CLA	C2B-C3B-CAB-CBB
24	BV	604	CLA	C2B-C3B-CAB-CBB
24	BV	610	CLA	C2B-C3B-CAB-CBB
24	Ba	311	CLA	C2B-C3B-CAB-CBB
24	Ba	312	CLA	C2B-C3B-CAB-CBB
24	BF	513	CLA	C2B-C3B-CAB-CBB
24	BU	614	CLA	C2B-C3B-CAB-CBB
27	Az	102	LHG	O2-C2-C3-O3
23	AA	302	CHL	CAA-CBA-CGA-O2A
24	7	312	CLA	CAA-CBA-CGA-O2A
33	F	102	HEM	CAD-CBD-CGD-O2D
24	B	602	CLA	C8-C10-C11-C12
24	BE	602	CLA	C13-C15-C16-C17
24	1	503	CLA	C8-C10-C11-C12
24	BU	602	CLA	C10-C11-C12-C13
23	Au	607	CHL	O1D-CGD-O2D-CED
27	b	622	LHG	C13-C14-C15-C16
27	BG	404	LHG	C12-C13-C14-C15
34	a	401	DGD	O1B-C1B-O2G-C2G
34	BD	401	DGD	O1B-C1B-O2G-C2G
24	N	611	CLA	C11-C12-C13-C14
27	C	520	LHG	C24-C25-C26-C27
27	BJ	618	LHG	C33-C34-C35-C36
26	S	616	NEX	C12-C13-C14-C15
26	n	617	NEX	C28-C29-C30-C31
26	BB	318	NEX	C28-C29-C30-C31
27	BF	520	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	d	405	LMG	O1-C7-C8-O7
30	A0	201	LMG	O7-C8-C9-O8
30	BG	405	LMG	O1-C7-C8-O7
30	I	101	LMG	C39-C40-C41-C42
24	b	610	CLA	C13-C15-C16-C17
24	5	602	CLA	C4C-C3C-CAC-CBC
26	7	319	NEX	C13-C14-C15-C35
29	K	101	BCR	C19-C20-C21-C22
29	b	601	BCR	C9-C10-C11-C12
29	f	101	BCR	C13-C14-C15-C16
29	Ay	101	BCR	C19-C20-C21-C22
29	BI	101	BCR	C13-C14-C15-C16
29	BK	101	BCR	C9-C10-C11-C12
24	S	612	CLA	C3-C5-C6-C7
23	7	302	CHL	CAA-CBA-CGA-O2A
23	7	307	CHL	CAA-CBA-CGA-O2A
27	g	618	LHG	C33-C34-C35-C36
27	BE	622	LHG	C13-C14-C15-C16
24	y	305	CLA	O1D-CGD-O2D-CED
27	Y	319	LHG	C29-C30-C31-C32
27	BQ	618	LHG	C34-C35-C36-C37
30	B	620	LMG	C38-C39-C40-C41
32	L	103	SQD	C30-C31-C32-C33
24	C	503	CLA	C8-C10-C11-C12
23	Au	609	CHL	C4C-C3C-CAC-CBC
24	c	512	CLA	O1A-CGA-O2A-C1
30	i	101	LMG	O10-C28-O8-C9
33	4	102	HEM	CAD-CBD-CGD-O2D
33	BI	102	HEM	CAA-CBA-CGA-O2A
32	A1	101	SQD	C30-C31-C32-C33
24	b	610	CLA	C4-C3-C5-C6
24	Ba	314	CLA	C4-C3-C5-C6
31	BG	403	PL9	C35-C34-C36-C37
23	G	606	CHL	C2-C1-O2A-CGA
23	g	606	CHL	C2-C1-O2A-CGA
23	Au	606	CHL	C2-C1-O2A-CGA
23	BJ	606	CHL	C2-C1-O2A-CGA
24	6	603	CLA	C2-C1-O2A-CGA
24	S	613	CLA	C2-C1-O2A-CGA
24	b	605	CLA	C2-C1-O2A-CGA
24	b	616	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	g	604	CLA	C2-C1-O2A-CGA
24	n	610	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
24	r	608	CLA	C2-C1-O2A-CGA
24	0	603	CLA	C2-C1-O2A-CGA
24	A6	613	CLA	C2-C1-O2A-CGA
24	BE	605	CLA	C2-C1-O2A-CGA
24	BE	616	CLA	C2-C1-O2A-CGA
24	BJ	604	CLA	C2-C1-O2A-CGA
24	BQ	610	CLA	C2-C1-O2A-CGA
24	BV	611	CLA	C2-C1-O2A-CGA
24	1	507	CLA	C2-C1-O2A-CGA
24	BF	513	CLA	C2-C1-O2A-CGA
24	BU	608	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C3-C5-C6
24	Ba	314	CLA	C2-C3-C5-C6
24	1	510	CLA	C2-C3-C5-C6
23	y	306	CHL	C2-C1-O2A-CGA
27	Y	319	LHG	C28-C29-C30-C31
30	c	501	LMG	C37-C38-C39-C40
23	7	307	CHL	CAA-CBA-CGA-O1A
33	f	102	HEM	CAA-CBA-CGA-O2A
23	Ba	306	CHL	C2-C1-O2A-CGA
27	6	617	LHG	C35-C36-C37-C38
27	Au	618	LHG	C30-C31-C32-C33
27	Ba	319	LHG	C11-C12-C13-C14
30	v	620	LMG	C38-C39-C40-C41
30	Aw	101	LMG	C39-C40-C41-C42
24	B	613	CLA	C11-C10-C8-C9
24	G	602	CLA	C11-C10-C8-C9
24	S	602	CLA	C6-C7-C8-C9
24	b	602	CLA	C14-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C14
24	y	303	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	v	613	CLA	C11-C10-C8-C9
24	Au	602	CLA	C14-C13-C15-C16
24	BE	604	CLA	C11-C12-C13-C14
24	Ba	303	CLA	C11-C10-C8-C9
24	1	512	CLA	C11-C10-C8-C9
27	BE	623	LHG	C24-C23-O8-C6
23	n	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	W	201	LHG	O10-C23-O8-C6
23	BB	306	CHL	C2-C1-O2A-CGA
27	BB	319	LHG	C35-C36-C37-C38
24	D	401	CLA	C3-C5-C6-C7
23	AA	307	CHL	CAA-CBA-CGA-O1A
23	Y	306	CHL	C2-C1-O2A-CGA
27	BB	319	LHG	C12-C13-C14-C15
27	Y	319	LHG	C2-C3-O3-P
38	A	409	PHO	C1A-C2A-CAA-CBA
38	a	409	PHO	C1A-C2A-CAA-CBA
38	R	408	PHO	C1A-C2A-CAA-CBA
38	BD	409	PHO	C1A-C2A-CAA-CBA
27	5	618	LHG	O8-C23-C24-C25
34	BK	102	DGD	O2G-C1B-C2B-C3B
30	BL	101	LMG	O10-C28-O8-C9
27	c	520	LHG	C25-C26-C27-C28
24	BB	312	CLA	C8-C10-C11-C12
24	1	503	CLA	C2A-CAA-CBA-CGA
23	8	304	CHL	CAA-CBA-CGA-O2A
23	A6	607	CHL	CAA-CBA-CGA-O2A
23	r	607	CHL	C4C-C3C-CAC-CBC
24	7	303	CLA	C4C-C3C-CAC-CBC
34	h	102	DGD	O1A-C1A-O1G-C1G
25	6	615	LUT	C1-C6-C7-C8
25	7	316	LUT	C1-C6-C7-C8
25	G	615	LUT	C1-C6-C7-C8
25	G	616	LUT	C5-C6-C7-C8
25	Y	316	LUT	C1-C6-C7-C8
25	y	317	LUT	C1-C6-C7-C8
25	r	615	LUT	C1-C6-C7-C8
25	AA	316	LUT	C1-C6-C7-C8
25	AB	311	LUT	C1-C6-C7-C8
25	Au	616	LUT	C5-C6-C7-C8
25	A2	615	LUT	C1-C6-C7-C8
25	Ba	317	LUT	C1-C6-C7-C8
25	BU	615	LUT	C1-C6-C7-C8
29	F	101	BCR	C23-C24-C25-C30
29	K	101	BCR	C23-C24-C25-C26
29	K	101	BCR	C23-C24-C25-C30
29	b	601	BCR	C1-C6-C7-C8
29	b	601	BCR	C23-C24-C25-C30
29	f	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
29	k	101	BCR	C23-C24-C25-C30
29	z	101	BCR	C23-C24-C25-C30
29	C	514	BCR	C23-C24-C25-C30
29	C	515	BCR	C1-C6-C7-C8
29	v	622	BCR	C23-C24-C25-C30
29	4	101	BCR	C23-C24-C25-C30
29	Ay	101	BCR	C23-C24-C25-C30
29	BE	601	BCR	C1-C6-C7-C8
29	BE	601	BCR	C23-C24-C25-C30
29	BI	101	BCR	C23-C24-C25-C30
29	BK	101	BCR	C1-C6-C7-C8
29	BN	101	BCR	C23-C24-C25-C30
29	1	514	BCR	C23-C24-C25-C30
29	1	515	BCR	C1-C6-C7-C8
29	BF	515	BCR	C23-C24-C25-C30
24	A2	603	CLA	C5-C6-C7-C8
24	BE	612	CLA	C5-C6-C7-C8
23	0	605	CHL	O1D-CGD-O2D-CED
23	G	608	CHL	CAA-CBA-CGA-O2A
34	h	102	DGD	O2G-C1B-C2B-C3B
30	C	501	LMG	C7-C8-C9-O8
30	1	501	LMG	C7-C8-C9-O8
24	6	612	CLA	CAA-CBA-CGA-O2A
24	AA	312	CLA	CAA-CBA-CGA-O1A
33	F	102	HEM	CAD-CBD-CGD-O1D
27	2	405	LHG	O1-C1-C2-C3
30	b	621	LMG	C38-C39-C40-C41
26	AA	319	NEX	C13-C14-C15-C35
29	k	101	BCR	C19-C20-C21-C22
29	BE	601	BCR	C9-C10-C11-C12
29	BN	101	BCR	C19-C20-C21-C22
24	c	512	CLA	CBA-CGA-O2A-C1
24	g	613	CLA	C4-C3-C5-C6
26	Au	617	NEX	C27-C28-C29-C30
26	Au	617	NEX	C31-C32-C33-C34
28	Au	619	XAT	C7-C8-C9-C10
24	BU	602	CLA	C8-C10-C11-C12
38	BD	408	PHO	C15-C16-C17-C18
23	A2	607	CHL	C2-C3-C5-C6
24	7	304	CLA	C2-C3-C5-C6
24	g	613	CLA	C2-C3-C5-C6
24	c	511	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	BF	511	CLA	C2-C3-C5-C6
23	Au	608	CHL	CAA-CBA-CGA-O2A
27	9	618	LHG	O8-C23-C24-C25
32	BO	102	SQD	C23-C24-C25-C26
23	e	601	CHL	CAA-CBA-CGA-O2A
24	BJ	610	CLA	C15-C16-C17-C18
27	c	519	LHG	C16-C17-C18-C19
27	BJ	618	LHG	C31-C32-C33-C34
34	a	413	DGD	O6D-C5D-C6D-O5D
34	BD	413	DGD	O6D-C5D-C6D-O5D
24	n	602	CLA	C10-C11-C12-C13
24	y	304	CLA	C5-C6-C7-C8
24	BQ	602	CLA	C10-C11-C12-C13
30	B	624	LMG	C8-C7-O1-C1
32	l	102	SQD	C45-C44-O6-C1
32	BO	102	SQD	C45-C44-O6-C1
23	BH	601	CHL	CAA-CBA-CGA-O2A
24	7	312	CLA	CAA-CBA-CGA-O1A
23	AA	308	CHL	O1A-CGA-O2A-C1
30	BE	621	LMG	C38-C39-C40-C41
32	Az	101	SQD	C24-C25-C26-C27
24	0	611	CLA	C6-C7-C8-C10
38	BD	409	PHO	C16-C17-C18-C20
24	C	508	CLA	C3-C5-C6-C7
30	c	501	LMG	C31-C32-C33-C34
24	v	611	CLA	C10-C11-C12-C13
24	v	613	CLA	C13-C15-C16-C17
24	BG	401	CLA	C13-C15-C16-C17
24	Ba	304	CLA	C5-C6-C7-C8
24	BF	503	CLA	C8-C10-C11-C12
24	S	602	CLA	C14-C13-C15-C16
24	Ba	305	CLA	O1D-CGD-O2D-CED
24	BE	606	CLA	C2A-CAA-CBA-CGA
24	b	614	CLA	C5-C6-C7-C8
27	D	404	LHG	C32-C33-C34-C35
27	y	319	LHG	C11-C12-C13-C14
34	c	516	DGD	C4A-C5A-C6A-C7A
23	6	609	CHL	C2C-C3C-CAC-CBC
27	B	621	LHG	C14-C15-C16-C17
24	BF	512	CLA	C3-C5-C6-C7
23	0	606	CHL	CAA-CBA-CGA-O2A
33	4	102	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	7	315	CLA	C4B-C3B-CAB-CBB
24	N	613	CLA	C4B-C3B-CAB-CBB
24	Y	311	CLA	C4B-C3B-CAB-CBB
24	b	606	CLA	C4B-C3B-CAB-CBB
24	b	613	CLA	C4B-C3B-CAB-CBB
24	g	610	CLA	C4B-C3B-CAB-CBB
24	n	604	CLA	C4B-C3B-CAB-CBB
24	y	311	CLA	C4B-C3B-CAB-CBB
24	c	504	CLA	C4B-C3B-CAB-CBB
24	c	513	CLA	C4B-C3B-CAB-CBB
24	c	514	CLA	C4B-C3B-CAB-CBB
24	2	403	CLA	C4B-C3B-CAB-CBB
24	A2	602	CLA	C4B-C3B-CAB-CBB
24	A6	609	CLA	C4B-C3B-CAB-CBB
24	BB	311	CLA	C4B-C3B-CAB-CBB
24	BE	613	CLA	C4B-C3B-CAB-CBB
24	BJ	610	CLA	C4B-C3B-CAB-CBB
24	BD	406	CLA	C4B-C3B-CAB-CBB
24	BF	513	CLA	C4B-C3B-CAB-CBB
24	BU	604	CLA	C4B-C3B-CAB-CBB
23	G	608	CHL	C4-C3-C5-C6
24	7	304	CLA	C4-C3-C5-C6
24	Au	612	CLA	C4-C3-C5-C6
24	BB	303	CLA	C4-C3-C5-C6
38	BD	409	PHO	C4-C3-C5-C6
32	BO	101	SQD	O49-C7-C8-C9
30	b	621	LMG	C15-C16-C17-C18
34	BF	517	DGD	C4A-C5A-C6A-C7A
23	g	607	CHL	C11-C12-C13-C15
23	n	609	CHL	C11-C12-C13-C15
23	BJ	607	CHL	C11-C12-C13-C15
23	BQ	609	CHL	C11-C12-C13-C15
24	B	609	CLA	C2-C3-C5-C6
24	D	401	CLA	C11-C10-C8-C7
24	N	602	CLA	C11-C10-C8-C7
24	N	612	CLA	C6-C7-C8-C10
24	s	609	CLA	C2-C3-C5-C6
24	y	314	CLA	C2-C3-C5-C6
24	AA	304	CLA	C2-C3-C5-C6
24	Aw	102	CLA	C12-C13-C15-C16
24	A2	611	CLA	C2-C3-C5-C6
24	A2	612	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	BE	608	CLA	C2-C3-C5-C6
24	BE	613	CLA	C6-C7-C8-C10
24	BJ	613	CLA	C2-C3-C5-C6
23	7	306	CHL	CAA-CBA-CGA-O2A
23	BV	607	CHL	CAA-CBA-CGA-O2A
30	v	620	LMG	C29-C28-O8-C9
30	BG	405	LMG	C15-C16-C17-C18
27	b	623	LHG	O1-C1-C2-O2
27	BQ	618	LHG	O1-C1-C2-O2
23	6	607	CHL	C3-C5-C6-C7
24	b	602	CLA	C15-C16-C17-C18
24	C	504	CLA	C13-C15-C16-C17
24	v	601	CLA	C15-C16-C17-C18
32	l	101	SQD	O49-C7-C8-C9
28	n	619	XAT	C13-C14-C15-C35
34	c	516	DGD	C2D-C1D-O3G-C3G
34	BF	517	DGD	C2D-C1D-O3G-C3G
23	n	608	CHL	C16-C17-C18-C19
24	BQ	611	CLA	C11-C12-C13-C15
27	1	520	LHG	C16-C17-C18-C19
30	d	405	LMG	C15-C16-C17-C18
30	BF	501	LMG	C37-C38-C39-C40
23	6	606	CHL	CAA-CBA-CGA-O2A
33	BI	102	HEM	CAA-CBA-CGA-O1A
27	y	319	LHG	C5-C4-O6-P
27	BB	319	LHG	C2-C3-O3-P
27	Ba	319	LHG	C5-C4-O6-P
30	C	501	LMG	O7-C8-C9-O8
30	c	501	LMG	O7-C8-C9-O8
30	1	501	LMG	O7-C8-C9-O8
30	BF	501	LMG	O7-C8-C9-O8
32	2	408	SQD	O47-C45-C46-O48
34	a	413	DGD	O2G-C2G-C3G-O3G
34	BD	413	DGD	O2G-C2G-C3G-O3G
32	l	102	SQD	C23-C24-C25-C26
32	Az	101	SQD	C23-C24-C25-C26
24	G	611	CLA	CBA-CGA-O2A-C1
30	2	407	LMG	C20-C21-C22-C23
24	1	513	CLA	C3-C5-C6-C7
23	AA	306	CHL	CAA-CBA-CGA-O2A
24	0	612	CLA	CAA-CBA-CGA-O2A
27	y	319	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	G	611	CLA	O1A-CGA-O2A-C1
23	Y	310	CHL	C2A-CAA-CBA-CGA
24	b	606	CLA	C2A-CAA-CBA-CGA
23	BU	607	CHL	C4C-C3C-CAC-CBC
23	7	308	CHL	C11-C12-C13-C14
24	6	611	CLA	C6-C7-C8-C10
30	BE	621	LMG	C4-C5-C6-O5
30	B	620	LMG	C29-C28-O8-C9
30	Aw	101	LMG	C29-C28-O8-C9
26	5	617	NEX	C39-C29-C30-C31
26	N	617	NEX	C39-C29-C30-C31
26	s	616	NEX	C20-C13-C14-C15
26	s	616	NEX	C39-C29-C30-C31
26	BQ	617	NEX	C39-C29-C30-C31
26	BV	616	NEX	C20-C13-C14-C15
26	BV	616	NEX	C39-C29-C30-C31
28	Au	619	XAT	C20-C13-C14-C15
29	BE	620	BCR	C16-C17-C18-C36
29	BN	101	BCR	C20-C21-C22-C37
32	L	101	SQD	C24-C25-C26-C27
24	Y	313	CLA	CAA-CBA-CGA-O2A
24	y	313	CLA	CAA-CBA-CGA-O2A
24	v	610	CLA	CAA-CBA-CGA-O2A
24	BB	313	CLA	CAA-CBA-CGA-O2A
23	Au	608	CHL	C4-C3-C5-C6
24	G	612	CLA	C4-C3-C5-C6
24	s	612	CLA	C4-C3-C5-C6
24	BE	615	CLA	C4-C3-C5-C6
24	R	404	CLA	C4-C3-C5-C6
24	1	507	CLA	C4-C3-C5-C6
31	D	403	PL9	C12-C11-C9-C10
24	B	601	CLA	C15-C16-C17-C18
24	B	611	CLA	C10-C11-C12-C13
24	B	613	CLA	C13-C15-C16-C17
30	b	621	LMG	C31-C32-C33-C34
24	Ba	305	CLA	CBD-CGD-O2D-CED
24	r	602	CLA	C10-C11-C12-C13
24	Ba	313	CLA	CAA-CBA-CGA-O2A
30	I	101	LMG	O7-C10-C11-C12
24	9	602	CLA	C12-C13-C15-C16
23	Y	309	CHL	C11-C12-C13-C14
24	D	402	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	G	610	CLA	C11-C10-C8-C9
24	b	607	CLA	C14-C13-C15-C16
24	b	609	CLA	C11-C12-C13-C14
24	d	401	CLA	C11-C10-C8-C9
24	d	402	CLA	C11-C12-C13-C14
24	g	602	CLA	C11-C10-C8-C9
24	g	611	CLA	C6-C7-C8-C9
24	y	304	CLA	C6-C7-C8-C9
24	y	312	CLA	C6-C7-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	c	511	CLA	C11-C10-C8-C9
24	r	602	CLA	C11-C10-C8-C9
24	v	605	CLA	C11-C10-C8-C9
24	v	607	CLA	C11-C10-C8-C9
24	2	403	CLA	C11-C12-C13-C14
24	Au	602	CLA	C11-C10-C8-C9
24	Au	610	CLA	C11-C10-C8-C9
24	BB	304	CLA	C14-C13-C15-C16
24	BE	607	CLA	C14-C13-C15-C16
24	BG	401	CLA	C11-C10-C8-C9
24	BG	402	CLA	C11-C12-C13-C14
24	BJ	611	CLA	C6-C7-C8-C9
24	BQ	602	CLA	C6-C7-C8-C9
24	Ba	304	CLA	C6-C7-C8-C9
24	Ba	304	CLA	C14-C13-C15-C16
24	1	510	CLA	C11-C10-C8-C9
24	BF	511	CLA	C11-C10-C8-C9
24	BU	602	CLA	C11-C10-C8-C9
24	8	302	CLA	CAA-CBA-CGA-O2A
23	G	606	CHL	C3A-C2A-CAA-CBA
23	n	606	CHL	C3A-C2A-CAA-CBA
23	y	302	CHL	C3A-C2A-CAA-CBA
23	Au	606	CHL	C3A-C2A-CAA-CBA
24	5	614	CLA	C3A-C2A-CAA-CBA
24	6	613	CLA	C3A-C2A-CAA-CBA
24	S	604	CLA	C3A-C2A-CAA-CBA
24	C	503	CLA	C3A-C2A-CAA-CBA
24	C	511	CLA	C3A-C2A-CAA-CBA
24	c	504	CLA	C3A-C2A-CAA-CBA
24	9	614	CLA	C3A-C2A-CAA-CBA
24	v	602	CLA	C3A-C2A-CAA-CBA
34	BF	518	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
24	b	612	CLA	O1A-CGA-O2A-C1
24	BE	612	CLA	O1A-CGA-O2A-C1
27	6	617	LHG	O10-C23-O8-C6
23	y	307	CHL	CAA-CBA-CGA-O2A
24	6	614	CLA	CAA-CBA-CGA-O2A
24	B	610	CLA	CAA-CBA-CGA-O2A
24	B	613	CLA	CAA-CBA-CGA-O2A
24	C	502	CLA	CAA-CBA-CGA-O2A
24	v	613	CLA	CAA-CBA-CGA-O2A
24	BE	614	CLA	CAA-CBA-CGA-O2A
34	1	518	DGD	O2G-C1B-C2B-C3B
24	BG	402	CLA	CBD-CGD-O2D-CED
27	6	617	LHG	C10-C11-C12-C13
23	S	601	CHL	CAA-CBA-CGA-O2A
23	A6	601	CHL	CAA-CBA-CGA-O2A
24	7	313	CLA	CAA-CBA-CGA-O2A
24	S	603	CLA	CAA-CBA-CGA-O2A
24	AA	313	CLA	CAA-CBA-CGA-O2A
33	f	102	HEM	CAA-CBA-CGA-O1A
23	8	306	CHL	CAD-CBD-CGD-O2D
23	N	606	CHL	CAD-CBD-CGD-O2D
23	S	607	CHL	CAD-CBD-CGD-O2D
23	Y	307	CHL	CAD-CBD-CGD-O2D
23	n	609	CHL	CAD-CBD-CGD-O2D
23	s	607	CHL	CAD-CBD-CGD-O2D
23	y	310	CHL	CAD-CBD-CGD-O2D
23	r	613	CHL	CAD-CBD-CGD-O2D
23	AB	304	CHL	CAD-CBD-CGD-O2D
23	AB	306	CHL	CAD-CBD-CGD-O2D
23	A2	606	CHL	CAD-CBD-CGD-O2D
23	A6	607	CHL	CAD-CBD-CGD-O2D
23	BV	607	CHL	CAD-CBD-CGD-O2D
23	BU	613	CHL	CAD-CBD-CGD-O2D
24	5	610	CLA	CAD-CBD-CGD-O2D
24	6	603	CLA	CAD-CBD-CGD-O2D
24	6	610	CLA	CAD-CBD-CGD-O2D
24	7	303	CLA	CAD-CBD-CGD-O2D
24	7	313	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	CAD-CBD-CGD-O2D
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	D	402	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	N	614	CLA	CAD-CBD-CGD-O2D
24	S	604	CLA	CAD-CBD-CGD-O2D
24	Y	313	CLA	CAD-CBD-CGD-O2D
24	b	603	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	s	604	CLA	CAD-CBD-CGD-O2D
24	s	609	CLA	CAD-CBD-CGD-O2D
24	s	611	CLA	CAD-CBD-CGD-O2D
24	y	311	CLA	CAD-CBD-CGD-O2D
24	A	410	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	a	405	CLA	CAD-CBD-CGD-O2D
24	a	406	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
24	9	610	CLA	CAD-CBD-CGD-O2D
24	9	613	CLA	CAD-CBD-CGD-O2D
24	0	610	CLA	CAD-CBD-CGD-O2D
24	AA	303	CLA	CAD-CBD-CGD-O2D
24	AA	312	CLA	CAD-CBD-CGD-O2D
24	AA	314	CLA	CAD-CBD-CGD-O2D
24	v	603	CLA	CAD-CBD-CGD-O2D
24	v	606	CLA	CAD-CBD-CGD-O2D
24	v	609	CLA	CAD-CBD-CGD-O2D
24	v	613	CLA	CAD-CBD-CGD-O2D
24	2	403	CLA	CAD-CBD-CGD-O2D
24	A2	610	CLA	CAD-CBD-CGD-O2D
24	A6	604	CLA	CAD-CBD-CGD-O2D
24	BB	313	CLA	CAD-CBD-CGD-O2D
24	BE	603	CLA	CAD-CBD-CGD-O2D
24	BE	607	CLA	CAD-CBD-CGD-O2D
24	BE	610	CLA	CAD-CBD-CGD-O2D
24	BV	604	CLA	CAD-CBD-CGD-O2D
24	BV	611	CLA	CAD-CBD-CGD-O2D
24	Ba	311	CLA	CAD-CBD-CGD-O2D
24	BD	405	CLA	CAD-CBD-CGD-O2D
24	BD	406	CLA	CAD-CBD-CGD-O2D
24	BF	503	CLA	CAD-CBD-CGD-O2D
24	BF	512	CLA	CAD-CBD-CGD-O2D
24	BF	513	CLA	CAD-CBD-CGD-O2D
24	BU	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	BU	609	CLA	CAD-CBD-CGD-O2D
38	A	408	PHO	CAD-CBD-CGD-O2D
38	a	408	PHO	CAD-CBD-CGD-O2D
38	R	407	PHO	CAD-CBD-CGD-O2D
38	BD	408	PHO	CAD-CBD-CGD-O2D
27	Au	618	LHG	C10-C11-C12-C13
26	BB	318	NEX	C9-C10-C11-C12
24	BB	304	CLA	C2A-CAA-CBA-CGA
24	n	613	CLA	C3-C5-C6-C7
24	BJ	602	CLA	C3-C5-C6-C7
27	A0	202	LHG	O10-C23-O8-C6
24	g	610	CLA	C15-C16-C17-C18
24	BU	601	CLA	C2C-C3C-CAC-CBC
27	g	618	LHG	C11-C12-C13-C14
24	y	305	CLA	CBD-CGD-O2D-CED
24	v	609	CLA	C13-C15-C16-C17
24	BE	602	CLA	C15-C16-C17-C18
24	R	409	CLA	C2-C1-O2A-CGA
23	6	605	CHL	CAA-CBA-CGA-O2A
23	s	601	CHL	CAA-CBA-CGA-O2A
23	0	605	CHL	CAA-CBA-CGA-O2A
24	AB	302	CLA	CAA-CBA-CGA-O2A
24	A6	603	CLA	CAA-CBA-CGA-O2A
24	c	505	CLA	C4C-C3C-CAC-CBC
34	c	517	DGD	C5A-C6A-C7A-C8A
24	s	602	CLA	CAA-CBA-CGA-O2A
24	BF	502	CLA	CAA-CBA-CGA-O2A
23	9	609	CHL	C4-C3-C5-C6
24	A	405	CLA	C4-C3-C5-C6
24	AA	304	CLA	C4-C3-C5-C6
24	BV	612	CLA	C4-C3-C5-C6
31	d	403	PL9	C35-C34-C36-C37
31	2	404	PL9	C12-C11-C9-C10
24	BE	605	CLA	C3-C5-C6-C7
24	BQ	613	CLA	C3-C5-C6-C7
23	6	606	CHL	CAA-CBA-CGA-O1A
23	8	304	CHL	CAA-CBA-CGA-O1A
23	e	601	CHL	CAA-CBA-CGA-O1A
23	AB	304	CHL	CAA-CBA-CGA-O2A
23	AB	307	CHL	CAA-CBA-CGA-O2A
23	A6	607	CHL	CAA-CBA-CGA-O1A
23	BV	601	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	A2	613	CLA	C2-C3-C5-C6
23	5	607	CHL	CAA-CBA-CGA-O2A
24	N	612	CLA	CAA-CBA-CGA-O2A
24	n	612	CLA	CAA-CBA-CGA-O2A
24	C	512	CLA	CAA-CBA-CGA-O2A
24	c	502	CLA	CAA-CBA-CGA-O2A
24	A2	612	CLA	CAA-CBA-CGA-O2A
24	1	512	CLA	CAA-CBA-CGA-O2A
27	r	618	LHG	O8-C23-C24-C25
30	Aw	101	LMG	O7-C10-C11-C12
38	R	408	PHO	CAA-CBA-CGA-O2A
27	C	520	LHG	C16-C17-C18-C19
27	BJ	618	LHG	C11-C12-C13-C14
25	7	316	LUT	C7-C8-C9-C10
25	Y	316	LUT	C7-C8-C9-C10
25	y	316	LUT	C7-C8-C9-C10
25	0	615	LUT	C7-C8-C9-C10
25	AA	316	LUT	C7-C8-C9-C10
25	Ba	316	LUT	C7-C8-C9-C10
26	G	617	NEX	C31-C32-C33-C34
26	9	617	NEX	C11-C12-C13-C14
28	G	619	XAT	C7-C8-C9-C10
29	b	601	BCR	C17-C18-C19-C20
24	5	602	CLA	C14-C13-C15-C16
24	9	602	CLA	C14-C13-C15-C16
27	B	622	LHG	C29-C30-C31-C32
38	A	408	PHO	C15-C16-C17-C18
28	Y	301	XAT	O24-C26-C27-C28
28	r	616	XAT	O4-C6-C7-C8
28	BB	301	XAT	O24-C26-C27-C28
28	BU	616	XAT	O4-C6-C7-C8
30	c	501	LMG	C7-C8-C9-O8
30	BF	501	LMG	C7-C8-C9-O8
23	8	305	CHL	CAA-CBA-CGA-O1A
23	8	307	CHL	CAA-CBA-CGA-O2A
23	BH	601	CHL	CAA-CBA-CGA-O1A
24	6	612	CLA	CAA-CBA-CGA-O1A
27	G	618	LHG	C10-C11-C12-C13
27	Y	319	LHG	C12-C13-C14-C15
23	r	606	CHL	O1A-CGA-O2A-C1
23	G	607	CHL	O1D-CGD-O2D-CED
24	6	604	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	BY	201	LHG	O6-C4-C5-O7
24	AA	304	CLA	C3-C5-C6-C7
23	Ba	307	CHL	CAA-CBA-CGA-O2A
24	b	614	CLA	CAA-CBA-CGA-O2A
24	0	614	CLA	CAA-CBA-CGA-O2A
24	BQ	612	CLA	CAA-CBA-CGA-O2A
24	1	502	CLA	CAA-CBA-CGA-O2A
27	1	520	LHG	C29-C30-C31-C32
32	L	101	SQD	C9-C10-C11-C12
32	Az	101	SQD	C9-C10-C11-C12
23	8	305	CHL	CAA-CBA-CGA-O2A
23	0	605	CHL	CAA-CBA-CGA-O1A
23	AB	305	CHL	CAA-CBA-CGA-O1A
23	BV	605	CHL	CAA-CBA-CGA-O1A
30	BF	501	LMG	C31-C32-C33-C34
24	BB	311	CLA	C10-C11-C12-C13
23	5	607	CHL	O2A-C1-C2-C3
23	r	607	CHL	O2A-C1-C2-C3
23	9	607	CHL	O2A-C1-C2-C3
23	BU	607	CHL	O2A-C1-C2-C3
24	B	615	CLA	O2A-C1-C2-C3
24	N	610	CLA	O2A-C1-C2-C3
24	s	610	CLA	O2A-C1-C2-C3
24	v	615	CLA	O2A-C1-C2-C3
24	A2	610	CLA	O2A-C1-C2-C3
24	BV	610	CLA	O2A-C1-C2-C3
27	Au	618	LHG	O10-C23-O8-C6
24	C	502	CLA	O1D-CGD-O2D-CED
23	g	608	CHL	C2C-C3C-CAC-CBC
23	A2	605	CHL	C2-C1-O2A-CGA
27	0	617	LHG	C10-C11-C12-C13
30	D	405	LMG	C20-C21-C22-C23
30	A	412	LMG	C38-C39-C40-C41
23	AA	308	CHL	CBA-CGA-O2A-C1
24	a	405	CLA	CBA-CGA-O2A-C1
24	Y	304	CLA	C2A-CAA-CBA-CGA
24	C	503	CLA	C2A-CAA-CBA-CGA
24	r	604	CLA	C2A-CAA-CBA-CGA
24	AA	303	CLA	C2A-CAA-CBA-CGA
24	BV	609	CLA	C2A-CAA-CBA-CGA
24	y	303	CLA	C8-C10-C11-C12
23	9	607	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	CAA-CBA-CGA-O2A
30	B	624	LMG	O8-C28-C29-C30
30	v	623	LMG	O8-C28-C29-C30
34	C	518	DGD	O2G-C1B-C2B-C3B
24	b	605	CLA	C3-C5-C6-C7
24	g	602	CLA	C3-C5-C6-C7
24	a	405	CLA	C3-C5-C6-C7
23	s	605	CHL	CAA-CBA-CGA-O1A
23	s	605	CHL	CAA-CBA-CGA-O2A
23	0	606	CHL	CAA-CBA-CGA-O1A
23	AB	304	CHL	CAA-CBA-CGA-O1A
23	AB	305	CHL	CAA-CBA-CGA-O2A
23	BV	605	CHL	CAA-CBA-CGA-O2A
24	7	313	CLA	CAA-CBA-CGA-O1A
24	S	603	CLA	CAA-CBA-CGA-O1A
24	0	612	CLA	CAA-CBA-CGA-O1A
24	AB	302	CLA	CAA-CBA-CGA-O1A
24	A6	603	CLA	CAA-CBA-CGA-O1A
23	AA	308	CHL	C11-C12-C13-C14
24	n	611	CLA	C11-C12-C13-C15
23	5	609	CHL	CHA-CBD-CGD-O2D
23	7	310	CHL	CHA-CBD-CGD-O1D
23	G	601	CHL	CHA-CBD-CGD-O1D
23	S	601	CHL	CHA-CBD-CGD-O2D
23	g	608	CHL	CHA-CBD-CGD-O2D
23	s	601	CHL	CHA-CBD-CGD-O1D
23	s	601	CHL	CHA-CBD-CGD-O2D
23	AA	302	CHL	CHA-CBD-CGD-O1D
23	AA	302	CHL	CHA-CBD-CGD-O2D
23	AA	310	CHL	CHA-CBD-CGD-O1D
23	Au	605	CHL	CHA-CBD-CGD-O1D
23	A6	601	CHL	CHA-CBD-CGD-O2D
23	BJ	601	CHL	CHA-CBD-CGD-O2D
23	BJ	608	CHL	CHA-CBD-CGD-O2D
23	BV	601	CHL	CHA-CBD-CGD-O1D
23	BV	601	CHL	CHA-CBD-CGD-O2D
24	5	602	CLA	CHA-CBD-CGD-O1D
24	5	602	CLA	CHA-CBD-CGD-O2D
24	5	603	CLA	CHA-CBD-CGD-O2D
24	5	604	CLA	CHA-CBD-CGD-O2D
24	6	602	CLA	CHA-CBD-CGD-O2D
24	6	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	8	303	CLA	CHA-CBD-CGD-O2D
24	8	310	CLA	CHA-CBD-CGD-O1D
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O1D
24	G	604	CLA	CHA-CBD-CGD-O1D
24	G	614	CLA	CHA-CBD-CGD-O1D
24	G	614	CLA	CHA-CBD-CGD-O2D
24	N	604	CLA	CHA-CBD-CGD-O2D
24	S	603	CLA	CHA-CBD-CGD-O2D
24	S	612	CLA	CHA-CBD-CGD-O1D
24	S	612	CLA	CHA-CBD-CGD-O2D
24	Y	304	CLA	CHA-CBD-CGD-O1D
24	b	602	CLA	CHA-CBD-CGD-O1D
24	b	602	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	613	CLA	CHA-CBD-CGD-O1D
24	g	614	CLA	CHA-CBD-CGD-O1D
24	n	602	CLA	CHA-CBD-CGD-O1D
24	n	602	CLA	CHA-CBD-CGD-O2D
24	n	603	CLA	CHA-CBD-CGD-O1D
24	n	603	CLA	CHA-CBD-CGD-O2D
24	n	604	CLA	CHA-CBD-CGD-O1D
24	n	604	CLA	CHA-CBD-CGD-O2D
24	s	602	CLA	CHA-CBD-CGD-O2D
24	s	603	CLA	CHA-CBD-CGD-O1D
24	s	603	CLA	CHA-CBD-CGD-O2D
24	y	305	CLA	CHA-CBD-CGD-O1D
24	y	305	CLA	CHA-CBD-CGD-O2D
24	A	405	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O1D
24	c	505	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	r	603	CLA	CHA-CBD-CGD-O2D
24	9	602	CLA	CHA-CBD-CGD-O1D
24	9	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	9	604	CLA	CHA-CBD-CGD-O2D
24	0	602	CLA	CHA-CBD-CGD-O2D
24	0	612	CLA	CHA-CBD-CGD-O1D
24	AB	303	CLA	CHA-CBD-CGD-O2D
24	AB	310	CLA	CHA-CBD-CGD-O1D
24	v	601	CLA	CHA-CBD-CGD-O1D
24	v	611	CLA	CHA-CBD-CGD-O2D
24	v	614	CLA	CHA-CBD-CGD-O1D
24	v	614	CLA	CHA-CBD-CGD-O2D
24	Au	604	CLA	CHA-CBD-CGD-O1D
24	Au	614	CLA	CHA-CBD-CGD-O1D
24	Au	614	CLA	CHA-CBD-CGD-O2D
24	A2	604	CLA	CHA-CBD-CGD-O2D
24	A6	603	CLA	CHA-CBD-CGD-O2D
24	A6	612	CLA	CHA-CBD-CGD-O1D
24	A6	612	CLA	CHA-CBD-CGD-O2D
24	BB	304	CLA	CHA-CBD-CGD-O1D
24	BE	602	CLA	CHA-CBD-CGD-O1D
24	BE	606	CLA	CHA-CBD-CGD-O2D
24	BE	613	CLA	CHA-CBD-CGD-O2D
24	BJ	614	CLA	CHA-CBD-CGD-O1D
24	BQ	602	CLA	CHA-CBD-CGD-O1D
24	BQ	602	CLA	CHA-CBD-CGD-O2D
24	BQ	603	CLA	CHA-CBD-CGD-O2D
24	BQ	604	CLA	CHA-CBD-CGD-O1D
24	BQ	604	CLA	CHA-CBD-CGD-O2D
24	BV	602	CLA	CHA-CBD-CGD-O2D
24	BV	603	CLA	CHA-CBD-CGD-O1D
24	BV	603	CLA	CHA-CBD-CGD-O2D
24	Ba	305	CLA	CHA-CBD-CGD-O1D
24	Ba	305	CLA	CHA-CBD-CGD-O2D
24	R	404	CLA	CHA-CBD-CGD-O2D
24	1	505	CLA	CHA-CBD-CGD-O2D
24	1	507	CLA	CHA-CBD-CGD-O1D
24	1	507	CLA	CHA-CBD-CGD-O2D
24	1	509	CLA	CHA-CBD-CGD-O2D
24	1	510	CLA	CHA-CBD-CGD-O2D
24	1	511	CLA	CHA-CBD-CGD-O2D
24	BF	504	CLA	CHA-CBD-CGD-O1D
24	BF	505	CLA	CHA-CBD-CGD-O1D
24	BF	510	CLA	CHA-CBD-CGD-O1D
24	BF	510	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	BF	511	CLA	CHA-CBD-CGD-O1D
24	BF	512	CLA	CHA-CBD-CGD-O2D
24	BF	513	CLA	CHA-CBD-CGD-O1D
24	BU	603	CLA	CHA-CBD-CGD-O1D
24	BU	603	CLA	CHA-CBD-CGD-O2D
24	BU	604	CLA	CHA-CBD-CGD-O2D
38	R	408	PHO	C5-C6-C7-C8
23	6	605	CHL	CAA-CBA-CGA-O1A
23	AA	306	CHL	CAA-CBA-CGA-O1A
23	AB	307	CHL	CAA-CBA-CGA-O1A
23	A6	601	CHL	CAA-CBA-CGA-O1A
23	BV	601	CHL	CAA-CBA-CGA-O1A
24	AA	313	CLA	CAA-CBA-CGA-O1A
23	5	609	CHL	C4-C3-C5-C6
24	g	610	CLA	CAA-CBA-CGA-O2A
24	BJ	610	CLA	CAA-CBA-CGA-O2A
27	C	521	LHG	O8-C23-C24-C25
27	BF	521	LHG	O8-C23-C24-C25
23	BJ	608	CHL	C2C-C3C-CAC-CBC
27	Ba	319	LHG	C12-C13-C14-C15
24	d	401	CLA	C13-C15-C16-C17
26	5	617	NEX	C28-C29-C30-C31
26	N	617	NEX	C28-C29-C30-C31
26	Y	318	NEX	C28-C29-C30-C31
26	s	616	NEX	C28-C29-C30-C31
26	A2	617	NEX	C28-C29-C30-C31
26	BQ	617	NEX	C28-C29-C30-C31
26	BV	616	NEX	C28-C29-C30-C31
23	8	307	CHL	CAA-CBA-CGA-O1A
23	S	601	CHL	CAA-CBA-CGA-O1A
24	8	302	CLA	CAA-CBA-CGA-O1A
30	d	405	LMG	C20-C21-C22-C23
30	i	101	LMG	C38-C39-C40-C41
32	a	412	SQD	C10-C11-C12-C13
32	2	408	SQD	C17-C18-C19-C20
24	b	609	CLA	C13-C15-C16-C17
24	B	611	CLA	CAA-CBA-CGA-O2A
24	Y	312	CLA	CAA-CBA-CGA-O2A
24	b	615	CLA	CAA-CBA-CGA-O2A
24	Au	610	CLA	CAA-CBA-CGA-O2A
24	BB	303	CLA	CAA-CBA-CGA-O2A
24	BE	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	BE	615	CLA	CAA-CBA-CGA-O2A
24	BF	513	CLA	CAA-CBA-CGA-O2A
27	BU	617	LHG	O8-C23-C24-C25
38	A	409	PHO	CAA-CBA-CGA-O2A
34	C	516	DGD	C4A-C5A-C6A-C7A
27	Y	319	LHG	O7-C5-C6-O8
27	2	405	LHG	O7-C5-C6-O8
30	b	621	LMG	O7-C8-C9-O8
32	L	101	SQD	C23-C24-C25-C26
23	BU	606	CHL	O1A-CGA-O2A-C1
33	F	102	HEM	C1A-C2A-CAA-CBA
33	4	102	HEM	C1A-C2A-CAA-CBA
30	BG	405	LMG	C20-C21-C22-C23
24	Ba	303	CLA	C8-C10-C11-C12
38	A	409	PHO	C5-C6-C7-C8
24	1	508	CLA	C3-C5-C6-C7
23	s	601	CHL	CAA-CBA-CGA-O1A
32	D	406	SQD	C17-C18-C19-C20
32	BO	101	SQD	C30-C31-C32-C33
32	BD	412	SQD	C10-C11-C12-C13
24	v	605	CLA	O1A-CGA-O2A-C1
24	b	617	CLA	CAA-CBA-CGA-O2A
24	y	312	CLA	CAA-CBA-CGA-O2A
24	v	611	CLA	CAA-CBA-CGA-O2A
24	v	616	CLA	CAA-CBA-CGA-O2A
24	BB	312	CLA	CAA-CBA-CGA-O2A
24	Ba	312	CLA	CAA-CBA-CGA-O2A
27	c	520	LHG	O8-C23-C24-C25
27	1	521	LHG	O8-C23-C24-C25
34	C	516	DGD	O2G-C1B-C2B-C3B
24	BE	611	CLA	C16-C17-C18-C20
24	1	511	CLA	C16-C17-C18-C20
23	7	306	CHL	CAA-CBA-CGA-O1A
27	n	618	LHG	O1-C1-C2-O2
27	BE	623	LHG	O1-C1-C2-O2
27	c	519	LHG	C25-C26-C27-C28
32	BO	102	SQD	C13-C14-C15-C16
23	A2	607	CHL	CBA-CGA-O2A-C1
24	BE	612	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	C3-C5-C6-C7
23	r	605	CHL	CAA-CBA-CGA-O2A
23	Ba	306	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	BE	617	CLA	CAA-CBA-CGA-O2A
27	C	520	LHG	C29-C30-C31-C32
23	G	608	CHL	C11-C12-C13-C15
23	r	605	CHL	C11-C12-C13-C15
23	A2	609	CHL	C11-C12-C13-C15
23	BU	605	CHL	C11-C12-C13-C15
24	G	612	CLA	C2-C3-C5-C6
24	S	602	CLA	C6-C7-C8-C10
24	b	605	CLA	C6-C7-C8-C10
24	C	507	CLA	C12-C13-C15-C16
24	C	513	CLA	C12-C13-C15-C16
24	c	508	CLA	C12-C13-C15-C16
24	2	402	CLA	C11-C10-C8-C7
24	A6	602	CLA	C11-C10-C8-C7
24	BE	605	CLA	C6-C7-C8-C10
24	BE	608	CLA	C6-C7-C8-C10
24	BE	610	CLA	C2-C3-C5-C6
38	R	407	PHO	C12-C13-C15-C16
38	BD	409	PHO	C6-C7-C8-C10
23	BQ	608	CHL	C16-C17-C18-C19
27	2	406	LHG	C12-C13-C14-C15
27	A2	618	LHG	C34-C35-C36-C37
30	v	620	LMG	O9-C10-O7-C8
30	BE	621	LMG	O9-C10-O7-C8
24	BE	609	CLA	C13-C15-C16-C17
23	y	306	CHL	CAA-CBA-CGA-O2A
24	B	614	CLA	CAA-CBA-CGA-O2A
24	B	616	CLA	CAA-CBA-CGA-O2A
24	G	610	CLA	CAA-CBA-CGA-O2A
27	BY	201	LHG	O7-C7-C8-C9
34	1	516	DGD	O2G-C1B-C2B-C3B
34	BD	413	DGD	O2G-C1B-C2B-C3B
33	4	102	HEM	CAA-CBA-CGA-O2A
23	g	608	CHL	C11-C12-C13-C14
23	r	605	CHL	C11-C12-C13-C14
23	A2	609	CHL	C11-C12-C13-C14
23	BB	309	CHL	C11-C12-C13-C14
23	BU	605	CHL	C11-C12-C13-C14
24	B	607	CLA	C11-C10-C8-C9
24	Y	304	CLA	C14-C13-C15-C16
24	y	304	CLA	C14-C13-C15-C16
24	C	511	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C14-C13-C15-C16
24	r	608	CLA	C6-C7-C8-C9
24	BE	602	CLA	C14-C13-C15-C16
24	BE	610	CLA	C14-C13-C15-C16
24	BF	508	CLA	C14-C13-C15-C16
24	BB	313	CLA	CAA-CBA-CGA-O1A
26	g	617	NEX	C29-C30-C31-C32
26	BJ	617	NEX	C29-C30-C31-C32
29	h	101	BCR	C9-C10-C11-C12
34	C	516	DGD	C6A-C7A-C8A-C9A
24	BJ	610	CLA	C2B-C3B-CAB-CBB
30	BF	501	LMG	C4-C5-C6-O5
24	a	405	CLA	O1A-CGA-O2A-C1
32	Az	101	SQD	C7-C8-C9-C10
30	A0	201	LMG	C38-C39-C40-C41
24	b	612	CLA	CBA-CGA-O2A-C1
24	v	605	CLA	CBA-CGA-O2A-C1
34	BF	517	DGD	O2G-C1B-C2B-C3B
32	A	413	SQD	C4-C5-C6-S
32	a	412	SQD	C4-C5-C6-S
32	2	408	SQD	C4-C5-C6-S
32	R	411	SQD	C4-C5-C6-S
32	BD	412	SQD	C4-C5-C6-S
38	a	409	PHO	C16-C17-C18-C20
24	8	309	CLA	O1D-CGD-O2D-CED
27	Y	319	LHG	C35-C36-C37-C38
27	v	621	LHG	C14-C15-C16-C17
23	s	607	CHL	CAA-CBA-CGA-O2A
24	BU	602	CLA	C2A-CAA-CBA-CGA
31	d	403	PL9	C46-C47-C48-C49
24	c	502	CLA	CAA-CBA-CGA-O1A
24	1	502	CLA	CAA-CBA-CGA-O1A
23	s	607	CHL	C4C-C3C-CAC-CBC
27	BE	623	LHG	C29-C30-C31-C32
24	b	611	CLA	CAA-CBA-CGA-O2A
24	y	311	CLA	C10-C11-C12-C13
23	N	605	CHL	C2-C1-O2A-CGA
27	BQ	618	LHG	C15-C16-C17-C18
32	l	101	SQD	C30-C31-C32-C33
23	5	606	CHL	CAA-CBA-CGA-O2A
24	BF	502	CLA	CAA-CBA-CGA-O1A
27	c	520	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	I	101	LMG	O9-C10-C11-C12
24	Y	311	CLA	C10-C11-C12-C13
24	n	603	CLA	C16-C17-C18-C20
24	1	507	CLA	C16-C17-C18-C20
24	0	613	CLA	C4-C3-C5-C6
24	BJ	613	CLA	C4-C3-C5-C6
38	A	409	PHO	C4-C3-C5-C6
24	v	609	CLA	C2-C3-C5-C6
24	Au	612	CLA	C2-C3-C5-C6
23	BV	607	CHL	CAA-CBA-CGA-O1A
24	N	612	CLA	CAA-CBA-CGA-O1A
24	0	614	CLA	CAA-CBA-CGA-O1A
25	BB	316	LUT	C7-C8-C9-C10
25	BJ	615	LUT	C7-C8-C9-C10
27	D	404	LHG	C26-C27-C28-C29
23	r	606	CHL	CBA-CGA-O2A-C1
23	BU	606	CHL	CBA-CGA-O2A-C1
24	BD	405	CLA	CBA-CGA-O2A-C1
27	n	618	LHG	C15-C16-C17-C18
23	8	307	CHL	C1A-C2A-CAA-CBA
23	N	606	CHL	C1A-C2A-CAA-CBA
23	s	605	CHL	C1A-C2A-CAA-CBA
23	y	302	CHL	C1A-C2A-CAA-CBA
23	Au	601	CHL	C1A-C2A-CAA-CBA
23	A2	606	CHL	C1A-C2A-CAA-CBA
23	BB	310	CHL	C1A-C2A-CAA-CBA
23	Ba	302	CHL	C1A-C2A-CAA-CBA
24	5	613	CLA	C1A-C2A-CAA-CBA
24	B	611	CLA	C1A-C2A-CAA-CBA
24	G	613	CLA	C1A-C2A-CAA-CBA
24	Y	314	CLA	C1A-C2A-CAA-CBA
24	g	611	CLA	C1A-C2A-CAA-CBA
24	g	614	CLA	C1A-C2A-CAA-CBA
24	C	503	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	9	613	CLA	C1A-C2A-CAA-CBA
24	v	611	CLA	C1A-C2A-CAA-CBA
24	Au	613	CLA	C1A-C2A-CAA-CBA
24	BB	314	CLA	C1A-C2A-CAA-CBA
24	BJ	611	CLA	C1A-C2A-CAA-CBA
24	BJ	614	CLA	C1A-C2A-CAA-CBA
24	BF	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	BE	622	LHG	C11-C12-C13-C14
32	l	101	SQD	C25-C26-C27-C28
24	B	607	CLA	C16-C17-C18-C20
24	1	511	CLA	C16-C17-C18-C19
24	Y	313	CLA	CAA-CBA-CGA-O1A
24	C	502	CLA	CAA-CBA-CGA-O1A
24	v	610	CLA	CAA-CBA-CGA-O1A
24	BE	617	CLA	CAA-CBA-CGA-O1A
27	BF	521	LHG	O10-C23-C24-C25
30	Aw	101	LMG	O9-C10-C11-C12
27	b	622	LHG	C11-C12-C13-C14
23	A2	607	CHL	O1A-CGA-O2A-C1
27	BE	624	LHG	O10-C23-O8-C6
24	S	611	CLA	C2-C1-O2A-CGA
24	s	613	CLA	C2-C1-O2A-CGA
24	A6	611	CLA	C2-C1-O2A-CGA
27	BF	520	LHG	C25-C26-C27-C28
24	C	502	CLA	C15-C16-C17-C18
30	I	101	LMG	C29-C28-O8-C9
24	6	614	CLA	CAA-CBA-CGA-O1A
24	g	610	CLA	CAA-CBA-CGA-O1A
24	C	512	CLA	CAA-CBA-CGA-O1A
24	A2	612	CLA	CAA-CBA-CGA-O1A
24	Ba	313	CLA	CAA-CBA-CGA-O1A
24	1	512	CLA	CAA-CBA-CGA-O1A
27	w	201	LHG	O9-C7-C8-C9
27	1	521	LHG	O10-C23-C24-C25
32	BO	101	SQD	C25-C26-C27-C28
34	1	516	DGD	C6A-C7A-C8A-C9A
33	F	102	HEM	CAA-CBA-CGA-O2A
23	Y	306	CHL	CAA-CBA-CGA-O2A
24	v	614	CLA	CAA-CBA-CGA-O2A
34	a	413	DGD	O2G-C1B-C2B-C3B
27	6	617	LHG	C27-C28-C29-C30
24	G	602	CLA	C2A-CAA-CBA-CGA
24	S	609	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA
24	r	602	CLA	C2A-CAA-CBA-CGA
24	Au	602	CLA	C2A-CAA-CBA-CGA
24	A6	609	CLA	C2A-CAA-CBA-CGA
24	BF	506	CLA	C2A-CAA-CBA-CGA
23	BB	302	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	BF	520	LHG	C32-C33-C34-C35
30	1	501	LMG	C37-C38-C39-C40
34	c	516	DGD	C6A-C7A-C8A-C9A
24	G	612	CLA	C11-C12-C13-C14
24	b	611	CLA	C16-C17-C18-C20
24	BF	508	CLA	C16-C17-C18-C20
24	G	610	CLA	CAA-CBA-CGA-O1A
24	y	313	CLA	CAA-CBA-CGA-O1A
24	BJ	610	CLA	CAA-CBA-CGA-O1A
27	BY	201	LHG	O9-C7-C8-C9
24	B	609	CLA	C13-C15-C16-C17
24	AB	308	CLA	CAA-CBA-CGA-O2A
30	BL	101	LMG	C38-C39-C40-C41
24	Y	303	CLA	C4-C3-C5-C6
24	y	314	CLA	C4-C3-C5-C6
23	BU	605	CHL	CAA-CBA-CGA-O2A
27	w	201	LHG	O7-C7-C8-C9
24	S	602	CLA	C3-C5-C6-C7
27	n	618	LHG	C2-C3-O3-P
27	BQ	618	LHG	C2-C3-O3-P
30	c	518	LMG	C28-C29-C30-C31
23	9	607	CHL	CAA-CBA-CGA-O1A
24	B	616	CLA	CAA-CBA-CGA-O1A
24	Au	610	CLA	CAA-CBA-CGA-O1A
27	C	521	LHG	O10-C23-C24-C25
27	N	618	LHG	C34-C35-C36-C37
24	5	612	CLA	CAA-CBA-CGA-O2A
24	BF	506	CLA	C13-C15-C16-C17
27	y	319	LHG	C28-C29-C30-C31
23	5	605	CHL	C4B-C3B-CAB-CBB
23	e	601	CHL	C4B-C3B-CAB-CBB
23	9	605	CHL	C4B-C3B-CAB-CBB
23	Ba	307	CHL	C4B-C3B-CAB-CBB
24	7	313	CLA	C4B-C3B-CAB-CBB
24	B	610	CLA	C4B-C3B-CAB-CBB
24	S	610	CLA	C4B-C3B-CAB-CBB
24	b	617	CLA	C4B-C3B-CAB-CBB
24	A2	613	CLA	C4B-C3B-CAB-CBB
24	BU	601	CLA	C4B-C3B-CAB-CBB
27	D	404	LHG	C4-O6-P-O5
27	c	519	LHG	C3-O3-P-O4
27	2	406	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
27	BG	404	LHG	C4-O6-P-O5
27	BF	520	LHG	C3-O3-P-O4
24	BQ	603	CLA	C16-C17-C18-C20
27	BQ	618	LHG	C31-C32-C33-C34
24	B	610	CLA	CAA-CBA-CGA-O1A
24	BB	312	CLA	CAA-CBA-CGA-O1A
24	BF	513	CLA	CAA-CBA-CGA-O1A
24	r	603	CLA	CAA-CBA-CGA-O2A
24	BE	612	CLA	CAA-CBA-CGA-O2A
24	BU	603	CLA	CAA-CBA-CGA-O2A
28	G	619	XAT	C20-C13-C14-C15
28	Y	301	XAT	C20-C13-C14-C15
30	C	501	LMG	C37-C38-C39-C40
24	9	612	CLA	CAA-CBA-CGA-O2A
25	N	615	LUT	C1-C6-C7-C8
25	n	615	LUT	C1-C6-C7-C8
25	Au	615	LUT	C1-C6-C7-C8
25	A6	615	LUT	C5-C6-C7-C8
25	BB	316	LUT	C1-C6-C7-C8
25	BQ	615	LUT	C1-C6-C7-C8
29	B	623	BCR	C23-C24-C25-C30
29	f	101	BCR	C23-C24-C25-C26
29	k	101	BCR	C23-C24-C25-C26
29	Ay	101	BCR	C23-C24-C25-C26
29	BI	101	BCR	C23-C24-C25-C26
29	BN	101	BCR	C23-C24-C25-C26
27	6	617	LHG	C25-C26-C27-C28
34	1	518	DGD	C8B-C9B-CAB-CBB
28	r	616	XAT	C26-C27-C28-C29
28	BU	616	XAT	C26-C27-C28-C29
24	c	513	CLA	CAA-CBA-CGA-O1A
24	v	613	CLA	CAA-CBA-CGA-O1A
24	BE	614	CLA	CAA-CBA-CGA-O1A
24	BD	405	CLA	O1A-CGA-O2A-C1
24	y	305	CLA	CAA-CBA-CGA-O2A
24	A2	610	CLA	CAA-CBA-CGA-O2A
24	BQ	602	CLA	CAA-CBA-CGA-O2A
24	Ba	314	CLA	CAA-CBA-CGA-O2A
32	L	101	SQD	O48-C23-C24-C25
34	BF	517	DGD	C6A-C7A-C8A-C9A
24	c	508	CLA	C16-C17-C18-C20
24	BE	611	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	2	406	LHG	C7-C8-C9-C10
24	5	614	CLA	C2A-CAA-CBA-CGA
24	c	506	CLA	C2A-CAA-CBA-CGA
23	5	607	CHL	CAA-CBA-CGA-O1A
24	Y	312	CLA	CAA-CBA-CGA-O1A
24	v	616	CLA	CAA-CBA-CGA-O1A
27	W	201	LHG	O9-C7-C8-C9
24	B	605	CLA	O1A-CGA-O2A-C1
24	c	503	CLA	C8-C10-C11-C12
34	R	401	DGD	C8A-C9A-CAA-CBA
34	BD	401	DGD	CAB-CBB-CCB-CDB
23	g	601	CHL	CAA-CBA-CGA-O2A
23	n	605	CHL	CAA-CBA-CGA-O2A
23	BJ	601	CHL	CAA-CBA-CGA-O2A
24	A6	602	CLA	CAA-CBA-CGA-O2A
32	Az	101	SQD	O48-C23-C24-C25
24	AB	309	CLA	O1D-CGD-O2D-CED
27	Ba	319	LHG	C28-C29-C30-C31
30	b	621	LMG	C39-C40-C41-C42
30	v	620	LMG	C21-C22-C23-C24
24	B	613	CLA	CAA-CBA-CGA-O1A
24	b	614	CLA	CAA-CBA-CGA-O1A
24	n	612	CLA	CAA-CBA-CGA-O1A
24	BQ	612	CLA	CAA-CBA-CGA-O1A
24	A6	612	CLA	C4-C3-C5-C6
24	1	502	CLA	C15-C16-C17-C18
24	C	503	CLA	C16-C17-C18-C20
24	8	308	CLA	CAA-CBA-CGA-O2A
23	7	310	CHL	CAD-CBD-CGD-O1D
23	AA	310	CHL	CAD-CBD-CGD-O1D
23	BU	613	CHL	CAD-CBD-CGD-O1D
24	6	611	CLA	CAD-CBD-CGD-O1D
24	6	612	CLA	CAD-CBD-CGD-O1D
24	7	304	CLA	C3-C5-C6-C7
24	7	305	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	N	604	CLA	CAD-CBD-CGD-O1D
24	N	611	CLA	CAD-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	CAD-CBD-CGD-O1D
24	n	611	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	512	CLA	CAD-CBD-CGD-O1D
24	9	603	CLA	CAD-CBD-CGD-O1D
24	0	611	CLA	CAD-CBD-CGD-O1D
24	0	612	CLA	CAD-CBD-CGD-O1D
24	AA	305	CLA	CAD-CBD-CGD-O1D
24	v	606	CLA	CAD-CBD-CGD-O1D
24	A2	604	CLA	CAD-CBD-CGD-O1D
24	A2	611	CLA	CAD-CBD-CGD-O1D
24	BE	613	CLA	CAD-CBD-CGD-O1D
24	BQ	611	CLA	CAD-CBD-CGD-O1D
24	1	503	CLA	CAD-CBD-CGD-O1D
24	BD	405	CLA	CAD-CBD-CGD-O1D
24	BF	504	CLA	CAD-CBD-CGD-O1D
32	L	101	SQD	C5-C6-S-O7
32	l	101	SQD	O5-C5-C6-S
32	l	102	SQD	C5-C6-S-O7
32	A	413	SQD	O5-C5-C6-S
32	a	412	SQD	O5-C5-C6-S
32	Az	101	SQD	O5-C5-C6-S
32	BO	101	SQD	O5-C5-C6-S
32	BO	102	SQD	C5-C6-S-O7
32	R	411	SQD	O5-C5-C6-S
32	BD	412	SQD	O5-C5-C6-S
34	Av	102	DGD	C1A-C2A-C3A-C4A
27	w	201	LHG	O10-C23-O8-C6
24	B	611	CLA	CAA-CBA-CGA-O1A
24	b	617	CLA	CAA-CBA-CGA-O1A
24	s	602	CLA	CAA-CBA-CGA-O1A
27	A0	202	LHG	O9-C7-C8-C9
32	A1	101	SQD	C25-C26-C27-C28
24	b	606	CLA	CAA-CBA-CGA-O2A
23	N	609	CHL	C11-C12-C13-C14
23	n	609	CHL	C11-C12-C13-C14
23	BJ	608	CHL	C11-C12-C13-C14
23	BQ	609	CHL	C11-C12-C13-C14
24	D	401	CLA	C11-C10-C8-C9
24	Y	314	CLA	C11-C10-C8-C9
24	A	410	CLA	C6-C7-C8-C9
24	v	603	CLA	C11-C12-C13-C14
24	2	402	CLA	C11-C10-C8-C9
24	BE	615	CLA	C11-C10-C8-C9
24	R	409	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	1	508	CLA	C14-C13-C15-C16
24	BF	504	CLA	C14-C13-C15-C16
24	BU	608	CLA	C6-C7-C8-C9
23	BV	607	CHL	C4C-C3C-CAC-CBC
24	A6	602	CLA	C14-C13-C15-C16
24	c	504	CLA	C10-C11-C12-C13
24	BE	603	CLA	C15-C16-C17-C18
24	b	615	CLA	CAA-CBA-CGA-O1A
24	y	312	CLA	CAA-CBA-CGA-O1A
32	BG	406	SQD	C12-C13-C14-C15
23	S	606	CHL	CAA-CBA-CGA-O2A
23	0	601	CHL	CAA-CBA-CGA-O2A
23	0	607	CHL	CAA-CBA-CGA-O2A
23	BQ	605	CHL	CAA-CBA-CGA-O2A
24	6	613	CLA	CAA-CBA-CGA-O2A
24	Y	303	CLA	CAA-CBA-CGA-O2A
24	y	314	CLA	CAA-CBA-CGA-O2A
24	c	504	CLA	CAA-CBA-CGA-O2A
24	A6	610	CLA	CAA-CBA-CGA-O2A
24	BE	606	CLA	CAA-CBA-CGA-O2A
27	v	621	LHG	O7-C7-C8-C9
27	A0	202	LHG	O7-C7-C8-C9
27	BE	622	LHG	O7-C7-C8-C9
32	l	102	SQD	O48-C23-C24-C25
32	2	408	SQD	O47-C7-C8-C9
24	c	513	CLA	C8-C10-C11-C12
23	5	606	CHL	CAA-CBA-CGA-O1A
24	s	608	CLA	CAA-CBA-CGA-O2A
33	4	102	HEM	CAA-CBA-CGA-O1A
27	Y	319	LHG	C10-C11-C12-C13
27	BB	319	LHG	C10-C11-C12-C13
24	v	611	CLA	CAA-CBA-CGA-O1A
27	BJ	618	LHG	C34-C35-C36-C37
34	H	102	DGD	C8A-C9A-CAA-CBA
24	7	303	CLA	C2A-CAA-CBA-CGA
24	9	614	CLA	C2A-CAA-CBA-CGA
24	0	610	CLA	C2A-CAA-CBA-CGA
34	a	401	DGD	CAB-CBB-CCB-CDB
23	6	607	CHL	CAA-CBA-CGA-O2A
23	A6	606	CHL	CAA-CBA-CGA-O2A
23	BV	606	CHL	CAA-CBA-CGA-O2A
24	Y	305	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	b	612	CLA	CAA-CBA-CGA-O2A
24	n	602	CLA	CAA-CBA-CGA-O2A
24	BB	305	CLA	CAA-CBA-CGA-O2A
27	B	621	LHG	O7-C7-C8-C9
32	d	406	SQD	O47-C7-C8-C9
32	BG	406	SQD	O47-C7-C8-C9
32	BO	102	SQD	O48-C23-C24-C25
27	G	618	LHG	O10-C23-O8-C6
24	9	611	CLA	CAA-CBA-CGA-O2A
27	n	618	LHG	C31-C32-C33-C34
34	1	517	DGD	CAA-CBA-CCA-CDA
24	A6	612	CLA	C3-C5-C6-C7
24	BE	611	CLA	CAA-CBA-CGA-O1A
24	Ba	312	CLA	CAA-CBA-CGA-O1A
24	C	503	CLA	C16-C17-C18-C19
27	g	618	LHG	C5-C4-O6-P
27	A2	618	LHG	C2-C3-O3-P
24	N	610	CLA	C4-C3-C5-C6
24	b	615	CLA	C4-C3-C5-C6
24	C	507	CLA	C4-C3-C5-C6
24	A2	613	CLA	C4-C3-C5-C6
38	a	409	PHO	C4-C3-C5-C6
24	0	613	CLA	C5-C6-C7-C8
30	c	501	LMG	C4-C5-C6-O5
23	6	601	CHL	C11-C12-C13-C15
23	G	608	CHL	C2-C3-C5-C6
23	N	609	CHL	C11-C12-C13-C15
23	r	607	CHL	C2-C3-C5-C6
23	Au	608	CHL	C11-C12-C13-C15
24	B	602	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	C6-C7-C8-C10
24	B	607	CLA	C6-C7-C8-C10
24	Y	303	CLA	C12-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C15
24	b	608	CLA	C6-C7-C8-C10
24	b	610	CLA	C2-C3-C5-C6
24	b	613	CLA	C6-C7-C8-C10
24	b	613	CLA	C12-C13-C15-C16
24	n	603	CLA	C6-C7-C8-C10
24	y	303	CLA	C12-C13-C15-C16
24	y	312	CLA	C11-C10-C8-C7
24	C	511	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C12-C13-C15-C16
24	c	514	CLA	C12-C13-C15-C16
24	r	608	CLA	C6-C7-C8-C10
24	AB	310	CLA	C3A-C2A-CAA-CBA
24	v	604	CLA	C6-C7-C8-C10
24	v	607	CLA	C6-C7-C8-C10
24	v	610	CLA	C11-C10-C8-C7
24	v	613	CLA	C6-C7-C8-C10
24	A2	602	CLA	C11-C10-C8-C7
24	BB	303	CLA	C12-C13-C15-C16
24	BE	604	CLA	C11-C12-C13-C15
24	BE	613	CLA	C12-C13-C15-C16
24	Ba	312	CLA	C11-C10-C8-C7
24	R	409	CLA	C6-C7-C8-C10
24	1	507	CLA	C12-C13-C15-C16
24	1	513	CLA	C12-C13-C15-C16
24	BF	504	CLA	C12-C13-C15-C16
24	BF	506	CLA	C12-C13-C15-C16
24	BF	508	CLA	C12-C13-C15-C16
24	BU	608	CLA	C6-C7-C8-C10
27	W	201	LHG	O6-C4-C5-O7
27	w	201	LHG	O6-C4-C5-O7
38	a	409	PHO	C6-C7-C8-C10
23	r	605	CHL	CAA-CBA-CGA-O1A
24	B	614	CLA	CAA-CBA-CGA-O1A
24	BB	303	CLA	CAA-CBA-CGA-O1A
32	2	408	SQD	O49-C7-C8-C9
24	5	611	CLA	CAA-CBA-CGA-O2A
24	5	612	CLA	CAA-CBA-CGA-O1A
23	6	601	CHL	CAA-CBA-CGA-O2A
23	BB	307	CHL	CAA-CBA-CGA-O2A
24	B	605	CLA	CAA-CBA-CGA-O2A
24	N	610	CLA	CAA-CBA-CGA-O2A
24	S	610	CLA	CAA-CBA-CGA-O2A
24	s	610	CLA	CAA-CBA-CGA-O2A
24	v	605	CLA	CAA-CBA-CGA-O2A
27	W	201	LHG	O7-C7-C8-C9
27	b	622	LHG	O7-C7-C8-C9
34	c	516	DGD	O2G-C1B-C2B-C3B
27	2	405	LHG	C29-C30-C31-C32
30	BE	621	LMG	C39-C40-C41-C42
32	BG	406	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	g	615	LUT	C7-C8-C9-C10
28	7	301	XAT	C7-C8-C9-C10
28	AA	301	XAT	C7-C8-C9-C10
23	s	606	CHL	CAA-CBA-CGA-O1A
23	0	607	CHL	CAA-CBA-CGA-O1A
23	BU	605	CHL	CAA-CBA-CGA-O1A
24	B	605	CLA	CAA-CBA-CGA-O1A
24	Y	305	CLA	CAA-CBA-CGA-O1A
24	BE	615	CLA	CAA-CBA-CGA-O1A
32	l	102	SQD	O10-C23-C24-C25
32	BO	102	SQD	O10-C23-C24-C25
23	7	309	CHL	CAA-CBA-CGA-O2A
27	BB	319	LHG	C18-C19-C20-C21
34	A	402	DGD	C8A-C9A-CAA-CBA
23	Y	307	CHL	CAA-CBA-CGA-O2A
23	s	606	CHL	CAA-CBA-CGA-O2A
23	BB	306	CHL	CAA-CBA-CGA-O2A
24	BV	610	CLA	CAA-CBA-CGA-O2A
27	0	617	LHG	O8-C23-C24-C25
27	Y	319	LHG	C18-C19-C20-C21
24	c	506	CLA	C13-C15-C16-C17
24	BB	303	CLA	C15-C16-C17-C18
27	BY	201	LHG	O10-C23-O8-C6
30	B	620	LMG	C21-C22-C23-C24
24	6	613	CLA	CAA-CBA-CGA-O1A
24	b	611	CLA	CAA-CBA-CGA-O1A
24	b	612	CLA	CAA-CBA-CGA-O1A
24	v	605	CLA	CAA-CBA-CGA-O1A
24	v	614	CLA	CAA-CBA-CGA-O1A
24	BB	305	CLA	CAA-CBA-CGA-O1A
27	L	102	LHG	O9-C7-C8-C9
27	Az	102	LHG	O9-C7-C8-C9
32	BG	406	SQD	O49-C7-C8-C9
24	B	605	CLA	CBA-CGA-O2A-C1
24	9	612	CLA	CAA-CBA-CGA-O1A
24	BV	608	CLA	CAA-CBA-CGA-O2A
23	BQ	605	CHL	O1A-CGA-O2A-C1
34	C	518	DGD	C8B-C9B-CAB-CBB
24	c	505	CLA	CAA-CBA-CGA-O2A
24	r	610	CLA	CAA-CBA-CGA-O2A
24	0	613	CLA	CAA-CBA-CGA-O2A
24	BF	504	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	BF	505	CLA	CAA-CBA-CGA-O2A
30	c	501	LMG	C21-C22-C23-C24
24	c	509	CLA	C10-C11-C12-C13
24	BF	509	CLA	C10-C11-C12-C13
23	6	601	CHL	CAA-CBA-CGA-O1A
23	6	607	CHL	CAA-CBA-CGA-O1A
23	0	601	CHL	CAA-CBA-CGA-O1A
34	a	413	DGD	O1B-C1B-C2B-C3B
34	BD	413	DGD	O1B-C1B-C2B-C3B
24	6	614	CLA	C2A-CAA-CBA-CGA
24	B	610	CLA	C2A-CAA-CBA-CGA
24	D	401	CLA	C2A-CAA-CBA-CGA
24	v	610	CLA	C2A-CAA-CBA-CGA
24	BE	611	CLA	C2A-CAA-CBA-CGA
24	1	503	CLA	C16-C17-C18-C19
24	8	301	CLA	CAA-CBA-CGA-O1A
24	8	301	CLA	CAA-CBA-CGA-O2A
24	AB	301	CLA	CAA-CBA-CGA-O2A
32	l	102	SQD	C13-C14-C15-C16
34	BK	102	DGD	CBB-CCB-CDB-CEB
24	BF	513	CLA	C8-C10-C11-C12
32	d	406	SQD	C12-C13-C14-C15
32	L	101	SQD	C7-C8-C9-C10
23	S	606	CHL	CAA-CBA-CGA-O1A
23	BV	606	CHL	CAA-CBA-CGA-O1A
24	S	610	CLA	CAA-CBA-CGA-O1A
24	Y	303	CLA	CAA-CBA-CGA-O1A
24	0	613	CLA	CAA-CBA-CGA-O1A
24	A6	610	CLA	CAA-CBA-CGA-O1A
24	Ba	312	CLA	C4-C3-C5-C6
23	n	601	CHL	CAA-CBA-CGA-O2A
23	BQ	601	CHL	CAA-CBA-CGA-O2A
27	6	617	LHG	O8-C23-C24-C25
23	AA	309	CHL	CAA-CBA-CGA-O2A
24	AB	301	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

699 monomers are involved in 2718 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	y	311	CLA	4	0
24	BU	604	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	Y	301	XAT	5	0
25	n	615	LUT	5	0
23	n	608	CHL	10	0
27	BQ	618	LHG	6	0
23	5	607	CHL	11	0
24	BU	601	CLA	3	0
29	B	618	BCR	1	0
29	BI	101	BCR	2	0
23	G	608	CHL	7	0
24	B	602	CLA	6	0
24	BJ	613	CLA	6	0
25	y	317	LUT	4	0
24	c	512	CLA	5	0
23	n	605	CHL	2	0
24	BU	614	CLA	1	0
32	A1	101	SQD	2	0
23	BB	306	CHL	5	0
23	AA	302	CHL	11	0
23	A6	601	CHL	2	0
24	n	612	CLA	3	0
23	n	609	CHL	15	0
28	AB	312	XAT	6	0
24	C	511	CLA	5	0
28	8	312	XAT	6	0
26	BB	318	NEX	3	0
24	AB	309	CLA	1	0
26	AA	319	NEX	4	0
24	8	309	CLA	1	0
34	h	102	DGD	4	0
38	a	408	PHO	4	0
26	BV	616	NEX	5	0
24	v	608	CLA	5	0
24	BV	610	CLA	2	0
25	S	614	LUT	4	0
28	BU	616	XAT	4	0
24	v	602	CLA	6	0
24	C	510	CLA	1	0
24	D	401	CLA	7	0
29	BN	101	BCR	2	0
30	C	501	LMG	2	0
24	S	609	CLA	4	0
29	8	313	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2	408	SQD	3	0
24	BE	603	CLA	13	0
23	BU	613	CHL	2	0
23	Au	609	CHL	8	0
23	7	309	CHL	5	0
29	C	514	BCR	2	0
27	C	520	LHG	2	0
24	Au	612	CLA	3	0
25	Ba	317	LUT	3	0
23	BJ	608	CHL	7	0
24	y	312	CLA	1	0
24	v	604	CLA	6	0
24	BU	608	CLA	3	0
25	Au	616	LUT	5	0
25	N	615	LUT	4	0
27	g	618	LHG	4	0
24	BJ	612	CLA	3	0
23	y	302	CHL	11	0
25	S	615	LUT	7	0
24	5	611	CLA	2	0
27	b	624	LHG	4	0
23	g	608	CHL	6	0
24	b	602	CLA	4	0
23	S	606	CHL	7	0
24	A2	610	CLA	6	0
23	9	606	CHL	5	0
27	A0	202	LHG	1	0
24	Y	311	CLA	5	0
23	A2	605	CHL	2	0
24	b	617	CLA	3	0
24	v	616	CLA	3	0
26	Ba	318	NEX	2	0
23	N	605	CHL	2	0
24	N	603	CLA	1	0
23	BJ	601	CHL	15	0
25	5	615	LUT	6	0
27	w	201	LHG	1	0
23	8	305	CHL	2	0
24	BB	312	CLA	3	0
24	g	604	CLA	2	0
27	BJ	618	LHG	4	0
24	B	616	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	603	CLA	4	0
27	BF	521	LHG	3	0
23	N	607	CHL	8	0
24	A2	614	CLA	3	0
24	BQ	610	CLA	12	0
23	9	601	CHL	6	0
30	1	519	LMG	3	0
38	A	409	PHO	2	0
24	BQ	612	CLA	4	0
27	9	618	LHG	3	0
29	AB	313	BCR	5	0
32	BD	412	SQD	6	0
23	Au	601	CHL	14	0
24	c	507	CLA	4	0
24	C	508	CLA	5	0
23	Y	309	CHL	5	0
29	R	410	BCR	1	0
24	R	404	CLA	5	0
24	BF	507	CLA	4	0
29	BF	515	BCR	4	0
23	Y	310	CHL	12	0
24	BE	602	CLA	5	0
24	AB	301	CLA	6	0
23	8	304	CHL	2	0
24	S	610	CLA	1	0
24	BU	603	CLA	3	0
25	A2	616	LUT	7	0
32	BO	101	SQD	5	0
24	BE	615	CLA	4	0
24	y	313	CLA	3	0
26	7	319	NEX	5	0
24	1	510	CLA	1	0
23	8	306	CHL	3	0
24	b	613	CLA	5	0
27	B	621	LHG	2	0
23	0	606	CHL	5	0
24	AB	302	CLA	2	0
25	5	616	LUT	9	0
24	r	614	CLA	3	0
23	y	308	CHL	6	0
23	g	609	CHL	16	0
24	n	610	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	608	CLA	5	0
29	1	514	BCR	3	0
25	r	615	LUT	9	0
30	1	501	LMG	2	0
30	A0	201	LMG	1	0
24	6	602	CLA	12	0
24	I	102	CLA	3	0
24	BV	604	CLA	6	0
24	Ba	303	CLA	2	0
24	c	503	CLA	1	0
23	r	605	CHL	17	0
24	5	614	CLA	1	0
24	Au	613	CLA	6	0
25	G	616	LUT	5	0
24	BE	613	CLA	4	0
24	5	602	CLA	8	0
24	v	605	CLA	9	0
24	R	405	CLA	6	0
24	BB	303	CLA	3	0
24	BE	617	CLA	3	0
27	c	520	LHG	3	0
34	a	401	DGD	2	0
24	s	610	CLA	3	0
24	1	511	CLA	3	0
23	7	302	CHL	9	0
24	g	610	CLA	2	0
24	7	304	CLA	5	0
24	BE	608	CLA	3	0
29	b	618	BCR	3	0
23	G	605	CHL	1	0
23	s	606	CHL	11	0
29	f	101	BCR	2	0
24	BV	603	CLA	1	0
24	Ba	311	CLA	4	0
24	C	505	CLA	3	0
33	BI	102	HEM	2	0
24	9	614	CLA	1	0
30	I	101	LMG	3	0
24	BD	407	CLA	3	0
24	A6	609	CLA	3	0
23	9	609	CHL	15	0
28	N	619	XAT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AA	314	CLA	3	0
25	N	616	LUT	6	0
23	AA	307	CHL	2	0
24	Ba	312	CLA	1	0
24	b	603	CLA	10	0
29	4	101	BCR	3	0
24	B	601	CLA	4	0
24	S	608	CLA	3	0
23	5	606	CHL	7	0
27	v	621	LHG	2	0
29	BE	618	BCR	4	0
24	b	616	CLA	4	0
34	C	517	DGD	4	0
24	Ba	305	CLA	2	0
30	BF	519	LMG	4	0
23	Au	608	CHL	6	0
25	6	615	LUT	8	0
24	A2	613	CLA	5	0
24	a	407	CLA	6	0
24	c	504	CLA	4	0
29	B	619	BCR	6	0
24	8	302	CLA	2	0
24	b	612	CLA	3	0
24	BF	504	CLA	2	0
38	BD	409	PHO	1	0
25	0	616	LUT	9	0
24	5	613	CLA	7	0
24	a	405	CLA	5	0
24	Au	611	CLA	3	0
27	n	618	LHG	5	0
30	BL	101	LMG	2	0
23	AB	305	CHL	2	0
23	G	606	CHL	3	0
23	BQ	607	CHL	10	0
34	c	517	DGD	4	0
24	N	610	CLA	9	0
28	Ba	301	XAT	2	0
31	BG	403	PL9	2	0
24	0	603	CLA	1	0
24	AB	310	CLA	2	0
24	BD	405	CLA	8	0
30	c	518	LMG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	610	CLA	2	0
23	g	601	CHL	14	0
25	Y	316	LUT	4	0
24	Y	313	CLA	1	0
24	A6	604	CLA	3	0
24	BV	608	CLA	6	0
24	BJ	602	CLA	6	0
23	0	607	CHL	6	0
24	BF	508	CLA	2	0
24	1	508	CLA	7	0
24	0	614	CLA	4	0
24	r	604	CLA	3	0
23	6	608	CHL	2	0
24	BQ	602	CLA	6	0
27	Au	618	LHG	4	0
26	5	617	NEX	1	0
23	AA	309	CHL	4	0
24	5	612	CLA	1	0
24	7	313	CLA	3	0
24	Aw	102	CLA	3	0
24	r	601	CLA	4	0
27	A2	618	LHG	3	0
29	c	515	BCR	3	0
24	s	604	CLA	6	0
24	A	410	CLA	1	0
27	BE	624	LHG	2	0
24	v	614	CLA	8	0
24	Y	314	CLA	5	0
33	f	102	HEM	2	0
24	A	406	CLA	5	0
23	BJ	607	CHL	10	0
24	N	602	CLA	2	0
23	A2	608	CHL	11	0
24	c	506	CLA	3	0
25	BV	615	LUT	4	0
26	9	617	NEX	1	0
24	BF	506	CLA	3	0
24	c	505	CLA	5	0
24	b	615	CLA	4	0
24	8	301	CLA	6	0
26	s	616	NEX	5	0
23	y	309	CHL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	7	307	CHL	2	0
27	L	102	LHG	3	0
24	0	610	CLA	10	0
24	BE	605	CLA	5	0
27	BG	404	LHG	1	0
27	BY	201	LHG	1	0
38	R	407	PHO	7	0
24	c	514	CLA	7	0
24	v	601	CLA	5	0
24	1	507	CLA	4	0
29	Av	101	BCR	4	0
32	d	406	SQD	3	0
23	BU	605	CHL	17	0
23	A2	609	CHL	10	0
26	Y	318	NEX	1	0
30	A	412	LMG	1	0
27	Az	102	LHG	3	0
24	y	305	CLA	2	0
29	Ay	102	BCR	5	0
23	g	607	CHL	8	0
24	G	610	CLA	4	0
27	N	618	LHG	5	0
24	0	613	CLA	10	0
24	BB	314	CLA	5	0
24	BJ	611	CLA	3	0
23	N	606	CHL	5	0
24	v	613	CLA	2	0
32	a	412	SQD	6	0
28	AA	318	XAT	3	0
24	BJ	604	CLA	2	0
23	r	613	CHL	3	0
24	9	610	CLA	9	0
27	6	617	LHG	5	0
24	d	402	CLA	1	0
30	C	519	LMG	3	0
24	v	615	CLA	4	0
24	BD	406	CLA	8	0
24	B	613	CLA	2	0
23	r	606	CHL	13	0
29	C	515	BCR	3	0
24	9	612	CLA	2	0
24	BU	612	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	0	611	CLA	6	0
23	Y	306	CHL	6	0
24	BF	511	CLA	5	0
24	y	304	CLA	3	0
24	Au	602	CLA	6	0
24	BQ	611	CLA	2	0
23	s	601	CHL	3	0
27	G	618	LHG	3	0
32	Az	101	SQD	3	0
23	y	310	CHL	12	0
24	8	303	CLA	2	0
24	BF	513	CLA	3	0
23	S	601	CHL	2	0
23	BV	607	CHL	5	0
23	BQ	605	CHL	2	0
23	8	307	CHL	4	0
23	BU	606	CHL	12	0
23	Ba	308	CHL	8	0
24	A2	612	CLA	1	0
24	C	509	CLA	2	0
24	7	312	CLA	2	0
26	r	617	NEX	5	0
24	BE	609	CLA	4	0
24	BG	402	CLA	1	0
29	BD	411	BCR	2	0
34	BF	518	DGD	4	0
24	Ba	313	CLA	2	0
29	F	101	BCR	1	0
26	n	617	NEX	3	0
27	Y	319	LHG	6	0
24	AA	303	CLA	11	0
26	N	617	NEX	3	0
24	Au	610	CLA	3	0
24	N	614	CLA	3	0
24	s	611	CLA	2	0
28	5	619	XAT	11	0
23	N	608	CHL	12	0
27	0	617	LHG	8	0
24	v	606	CLA	9	0
28	9	619	XAT	11	0
25	BV	614	LUT	6	0
36	BD	403	OEX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	r	602	CLA	10	0
23	5	605	CHL	2	0
24	5	603	CLA	3	0
29	z	101	BCR	5	0
24	g	611	CLA	3	0
24	C	507	CLA	2	0
24	A2	602	CLA	2	0
27	D	404	LHG	3	0
29	z	102	BCR	3	0
23	0	601	CHL	12	0
24	C	502	CLA	3	0
23	Y	307	CHL	5	0
25	BQ	616	LUT	6	0
24	S	612	CLA	1	0
38	A	408	PHO	6	0
29	v	622	BCR	5	0
28	BB	301	XAT	6	0
24	BE	612	CLA	3	0
24	v	610	CLA	2	0
24	b	610	CLA	12	0
24	AA	311	CLA	4	0
23	0	608	CHL	2	0
23	G	609	CHL	18	0
24	s	603	CLA	1	0
24	7	303	CLA	8	0
24	G	612	CLA	3	0
24	G	611	CLA	4	0
24	AA	304	CLA	4	0
24	s	602	CLA	6	0
23	A2	601	CHL	9	0
24	b	614	CLA	2	0
24	Y	315	CLA	1	0
32	BO	102	SQD	1	0
23	S	605	CHL	1	0
34	Av	102	DGD	6	0
24	S	602	CLA	8	0
25	BJ	615	LUT	7	0
34	H	102	DGD	6	0
25	AA	316	LUT	7	0
34	A	402	DGD	2	0
24	BD	410	CLA	1	0
24	d	401	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	502	CLA	2	0
28	BJ	619	XAT	1	0
24	BV	611	CLA	2	0
29	B	623	BCR	8	0
24	C	512	CLA	3	0
27	b	623	LHG	2	0
30	Aw	101	LMG	1	0
24	BB	311	CLA	3	0
23	7	308	CHL	6	0
24	v	609	CLA	12	0
24	b	609	CLA	5	0
24	9	603	CLA	4	0
28	BQ	619	XAT	5	0
25	6	616	LUT	9	0
24	9	602	CLA	7	0
25	y	316	LUT	5	0
26	A6	616	NEX	2	0
24	c	509	CLA	5	0
24	BF	512	CLA	3	0
24	s	608	CLA	6	0
23	5	609	CHL	15	0
24	BF	509	CLA	9	0
28	AA	301	XAT	3	0
24	g	602	CLA	5	0
25	BB	317	LUT	6	0
24	B	609	CLA	11	0
24	8	308	CLA	7	0
23	AB	307	CHL	8	0
29	H	101	BCR	5	0
23	6	606	CHL	7	0
24	c	513	CLA	3	0
24	N	613	CLA	5	0
24	y	314	CLA	3	0
24	6	613	CLA	11	0
25	Y	317	LUT	5	0
24	C	504	CLA	2	0
23	n	601	CHL	12	0
24	1	512	CLA	2	0
25	AB	311	LUT	9	0
28	n	619	XAT	2	0
26	BQ	617	NEX	3	0
24	0	612	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	G	617	NEX	1	0
24	B	606	CLA	8	0
31	2	404	PL9	1	0
34	1	518	DGD	2	0
27	Ba	319	LHG	4	0
24	N	612	CLA	1	0
23	BB	308	CHL	9	0
33	F	102	HEM	1	0
24	B	612	CLA	3	0
32	D	406	SQD	1	0
34	BD	401	DGD	2	0
23	BJ	605	CHL	3	0
23	g	606	CHL	7	0
23	Ba	309	CHL	8	0
24	6	612	CLA	3	0
24	9	613	CLA	7	0
26	BB	320	NEX	5	0
27	C	521	LHG	3	0
23	Ba	310	CHL	12	0
27	d	404	LHG	1	0
26	y	318	NEX	3	0
24	BU	602	CLA	12	0
32	R	411	SQD	9	0
23	BQ	608	CHL	9	0
23	BV	606	CHL	10	0
24	BV	602	CLA	4	0
30	BF	501	LMG	1	0
25	g	615	LUT	7	0
24	n	611	CLA	2	0
24	BQ	603	CLA	1	0
24	BB	315	CLA	1	0
24	c	511	CLA	3	0
23	0	609	CHL	12	0
25	AA	317	LUT	7	0
32	L	103	SQD	2	0
23	Au	607	CHL	10	0
24	BQ	614	CLA	2	0
23	BV	601	CHL	3	0
24	9	611	CLA	2	0
24	2	403	CLA	1	0
34	a	413	DGD	1	0
23	A6	607	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	y	306	CHL	3	0
24	1	513	CLA	7	0
23	A2	607	CHL	11	0
29	BE	620	BCR	5	0
24	b	611	CLA	6	0
24	A	405	CLA	6	0
24	AA	313	CLA	2	0
28	7	301	XAT	3	0
24	C	506	CLA	5	0
24	g	612	CLA	3	0
23	BB	302	CHL	14	0
24	S	604	CLA	3	0
24	n	614	CLA	2	0
24	9	604	CLA	5	0
24	A6	602	CLA	5	0
24	n	603	CLA	1	0
23	N	601	CHL	10	0
23	AA	308	CHL	7	0
24	AA	312	CLA	1	0
34	1	516	DGD	1	0
26	g	617	NEX	1	0
24	2	402	CLA	7	0
24	Y	303	CLA	3	0
24	r	610	CLA	3	0
23	BB	309	CHL	7	0
25	7	317	LUT	7	0
26	S	616	NEX	3	0
25	7	316	LUT	6	0
24	r	612	CLA	4	0
23	6	609	CHL	13	0
25	n	616	LUT	6	0
24	v	607	CLA	5	0
28	Au	619	XAT	4	0
27	y	319	LHG	5	0
24	C	513	CLA	6	0
27	r	618	LHG	6	0
23	S	607	CHL	6	0
24	s	609	CLA	4	0
29	1	515	BCR	4	0
24	A2	611	CLA	3	0
24	C	503	CLA	1	0
25	BB	316	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AB	304	CHL	3	0
23	G	601	CHL	13	0
24	6	614	CLA	4	0
24	b	604	CLA	1	0
27	1	521	LHG	3	0
30	i	101	LMG	2	0
29	Bb	101	BCR	3	0
32	A	413	SQD	8	0
29	B	617	BCR	6	0
24	c	508	CLA	5	0
25	8	311	LUT	6	0
26	BJ	617	NEX	1	0
24	0	604	CLA	2	0
32	BG	406	SQD	4	0
23	n	607	CHL	10	0
23	y	307	CHL	7	0
24	Ba	304	CLA	3	0
23	5	608	CHL	4	0
30	c	501	LMG	3	0
25	s	615	LUT	9	0
29	Ay	101	BCR	3	0
23	9	607	CHL	8	0
24	A	407	CLA	3	0
24	r	609	CLA	6	0
23	9	608	CHL	4	0
23	s	607	CHL	4	0
24	6	604	CLA	6	0
24	BU	610	CLA	3	0
24	n	602	CLA	5	0
25	Ba	316	LUT	4	0
27	1	520	LHG	1	0
29	b	601	BCR	7	0
24	BF	514	CLA	7	0
24	BE	611	CLA	3	0
24	R	406	CLA	2	0
29	v	617	BCR	5	0
24	Y	312	CLA	6	0
24	b	606	CLA	5	0
24	A2	604	CLA	1	0
24	BE	604	CLA	1	0
23	AB	306	CHL	3	0
24	BJ	610	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	G	619	XAT	4	0
29	b	619	BCR	3	0
34	R	401	DGD	2	0
24	y	303	CLA	3	0
24	s	612	CLA	1	0
23	Y	302	CHL	12	0
30	b	621	LMG	1	0
23	BB	310	CHL	10	0
27	5	618	LHG	3	0
23	Ba	302	CHL	10	0
24	BB	305	CLA	1	0
25	s	614	LUT	7	0
25	G	615	LUT	6	0
24	8	310	CLA	2	0
23	A6	606	CHL	7	0
24	n	613	CLA	5	0
24	BE	614	CLA	2	0
23	BB	307	CHL	4	0
24	G	603	CLA	1	0
28	g	619	XAT	1	0
24	5	604	CLA	6	0
31	D	403	PL9	1	0
24	BE	606	CLA	5	0
23	BJ	606	CHL	6	0
33	4	102	HEM	3	0
24	BQ	613	CLA	4	0
24	Ba	314	CLA	7	0
24	1	504	CLA	2	0
23	g	605	CHL	3	0
24	g	603	CLA	2	0
27	BE	623	LHG	1	0
30	BE	621	LMG	1	0
24	6	610	CLA	5	0
24	a	410	CLA	1	0
23	AA	310	CHL	10	0
24	b	607	CLA	9	0
29	A	411	BCR	3	0
24	a	406	CLA	7	0
23	s	605	CHL	5	0
24	5	610	CLA	13	0
36	a	403	OEX	1	0
32	l	101	SQD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	608	CLA	3	0
25	A6	615	LUT	8	0
24	1	505	CLA	2	0
25	Au	615	LUT	7	0
24	r	603	CLA	1	0
24	BE	610	CLA	11	0
25	A2	615	LUT	5	0
24	B	605	CLA	10	0
24	BB	313	CLA	2	0
23	Au	606	CHL	2	0
24	r	608	CLA	2	0
23	BQ	606	CHL	7	0
38	BD	408	PHO	5	0
23	A2	606	CHL	5	0
23	r	607	CHL	10	0
23	Ba	306	CHL	3	0
24	BV	609	CLA	7	0
24	AA	305	CLA	4	0
24	B	607	CLA	2	0
24	c	510	CLA	2	0
24	B	615	CLA	4	0
24	6	611	CLA	5	0
24	A6	608	CLA	2	0
24	BJ	603	CLA	3	0
24	1	503	CLA	1	0
25	9	615	LUT	8	0
23	n	606	CHL	8	0
23	BQ	601	CHL	11	0
24	N	611	CLA	3	0
25	BU	615	LUT	10	0
32	l	102	SQD	2	0
29	h	101	BCR	7	0
23	9	605	CHL	2	0
24	G	602	CLA	4	0
24	1	506	CLA	5	0
24	BF	505	CLA	2	0
24	B	611	CLA	5	0
24	v	603	CLA	3	0
24	BF	510	CLA	3	0
27	2	405	LHG	1	0
31	d	403	PL9	3	0
23	BV	605	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	604	CLA	6	0
28	r	616	XAT	5	0
24	v	611	CLA	5	0
23	BU	607	CHL	12	0
23	6	601	CHL	16	0
25	A6	614	LUT	2	0
26	A2	617	NEX	3	0
24	BV	612	CLA	1	0
24	Y	304	CLA	2	0
26	Au	617	NEX	1	0
29	K	102	BCR	2	0
24	BU	609	CLA	5	0
23	7	310	CHL	11	0
24	AB	308	CLA	11	0
28	A2	619	XAT	6	0
24	BG	401	CLA	7	0
34	C	518	DGD	1	0
25	BJ	616	LUT	10	0
29	a	411	BCR	3	0
24	A2	603	CLA	3	0
23	G	607	CHL	11	0
29	BF	516	BCR	2	0
24	6	603	CLA	1	0
23	Y	308	CHL	9	0
23	BQ	609	CHL	15	0
24	7	311	CLA	4	0
23	5	601	CHL	5	0
24	1	509	CLA	1	0
24	B	614	CLA	7	0
25	9	616	LUT	10	0
29	k	101	BCR	1	0
32	L	101	SQD	3	0
24	7	314	CLA	3	0
24	BE	616	CLA	2	0
28	y	301	XAT	3	0
24	BE	607	CLA	8	0
25	g	616	LUT	9	0
25	0	615	LUT	10	0
24	BB	304	CLA	1	0
29	BK	101	BCR	8	0
23	Ba	307	CHL	6	0
23	N	609	CHL	9	0

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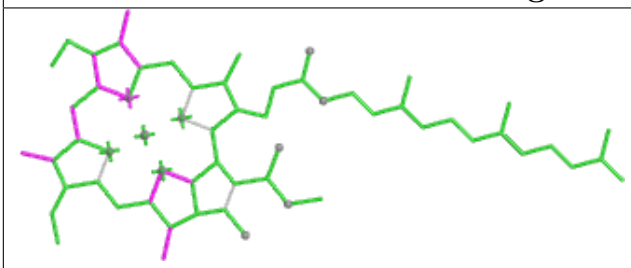
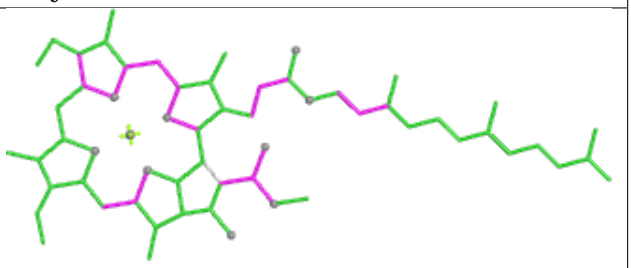
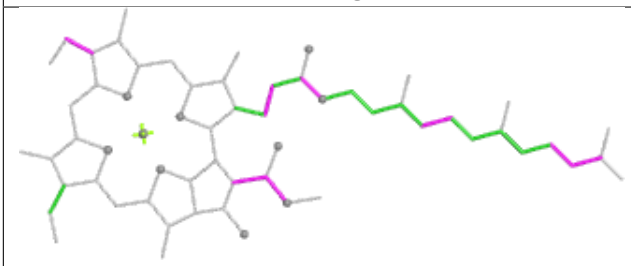
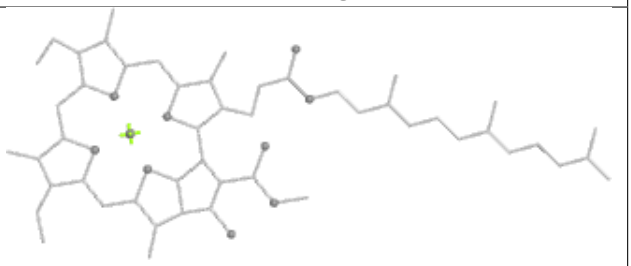
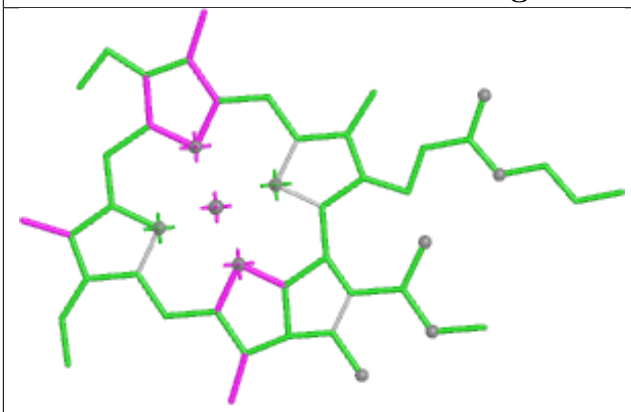
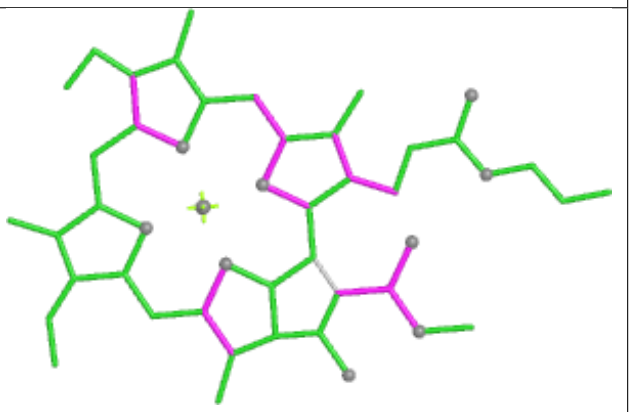
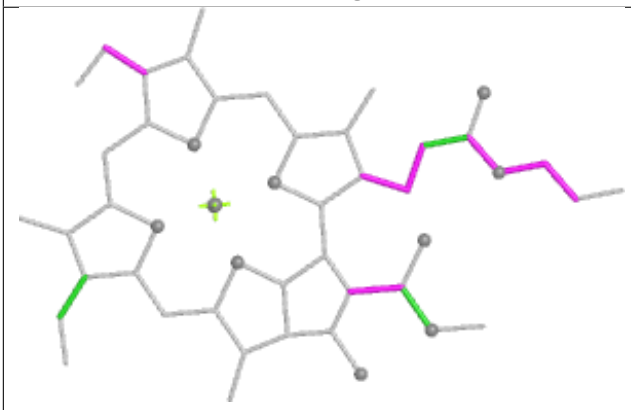
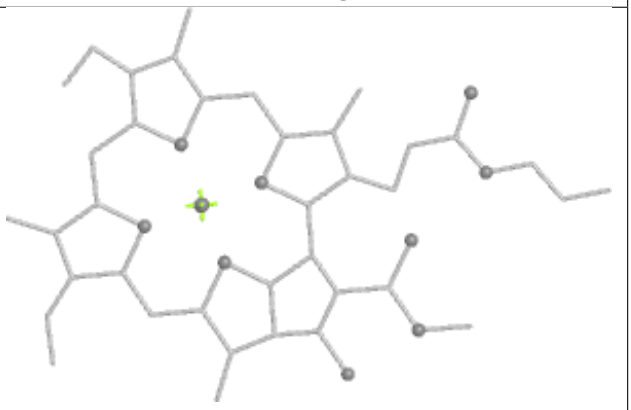
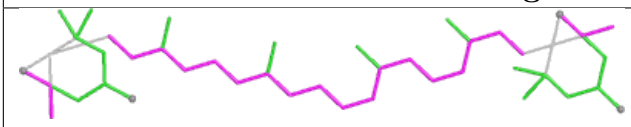
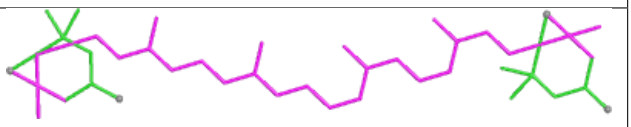
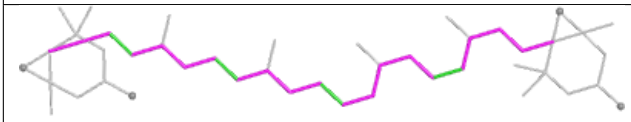
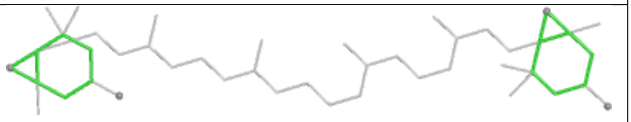
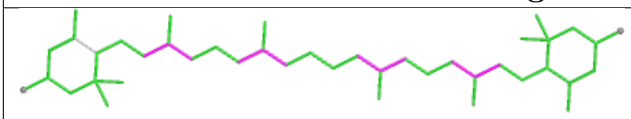
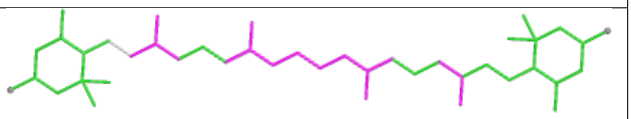
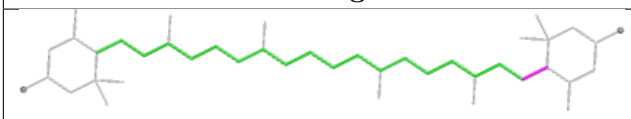
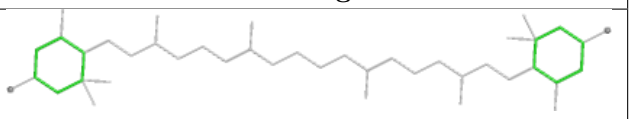
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A6	610	CLA	1	0
29	b	620	BCR	3	0
24	G	613	CLA	6	0
24	v	612	CLA	4	0
27	BB	319	LHG	7	0
24	r	611	CLA	1	0
27	BU	617	LHG	5	0
27	W	201	LHG	1	0
34	BK	102	DGD	6	0
34	1	517	DGD	4	0
24	0	602	CLA	5	0
24	c	502	CLA	4	0
24	7	305	CLA	4	0
24	AB	303	CLA	3	0
24	BF	502	CLA	2	0
24	g	613	CLA	5	0
28	7	318	XAT	1	0
23	BJ	609	CHL	15	0
29	K	101	BCR	3	0
25	BQ	615	LUT	5	0
29	BE	601	BCR	6	0
23	6	607	CHL	7	0
24	b	605	CLA	6	0
29	v	619	BCR	6	0
23	A6	605	CHL	1	0

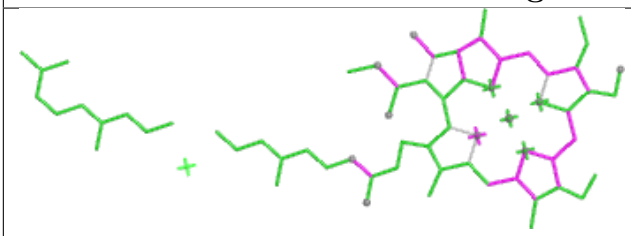
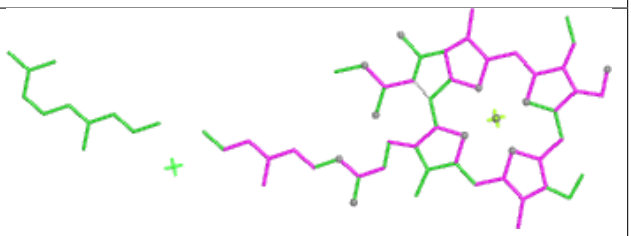
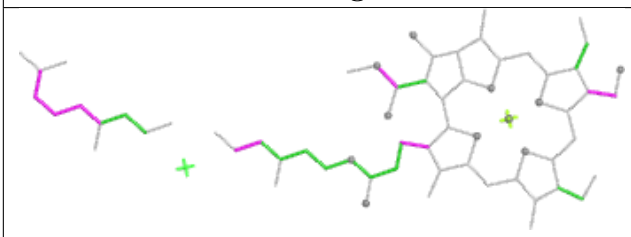
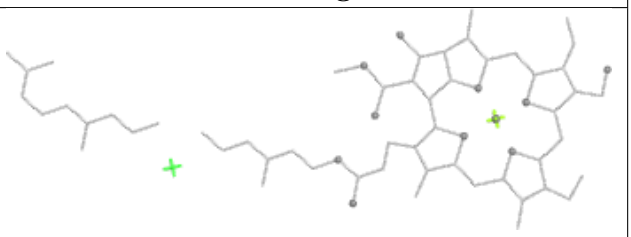
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA y 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

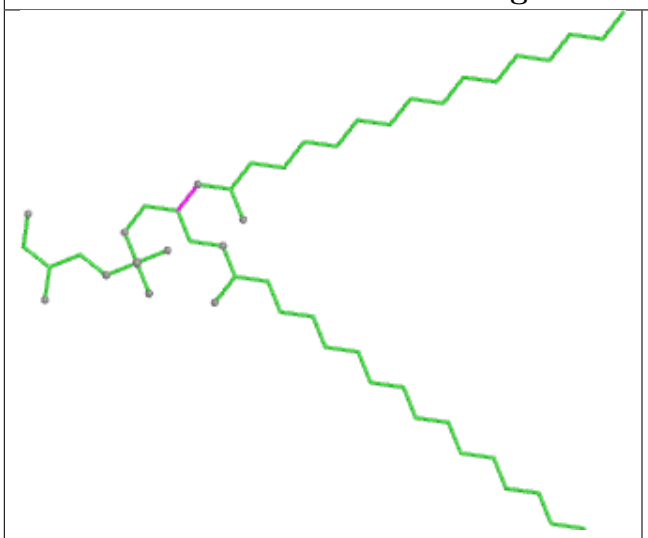
Ligand CLA BU 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT Y 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

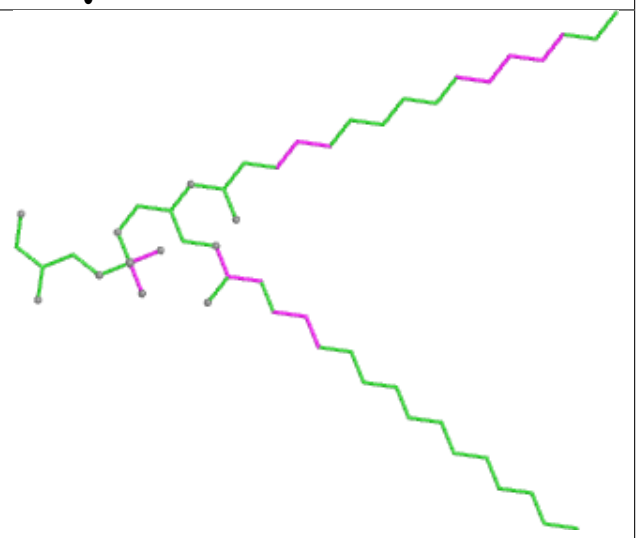
Ligand LUT n 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL n 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

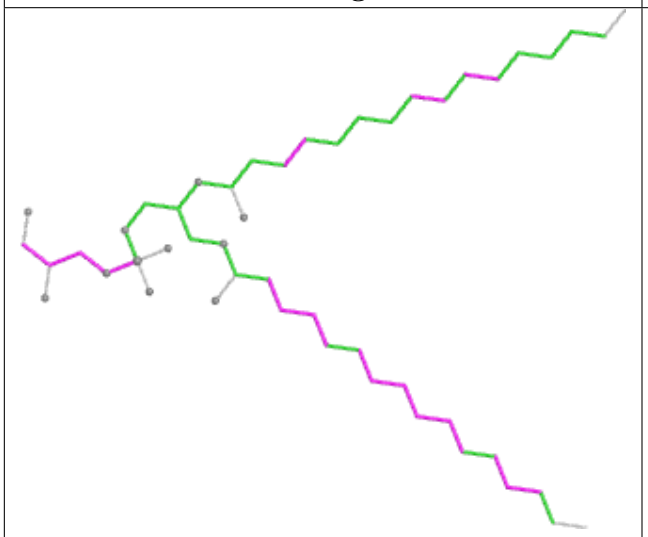
Ligand LHG BQ 618



Bond lengths



Bond angles



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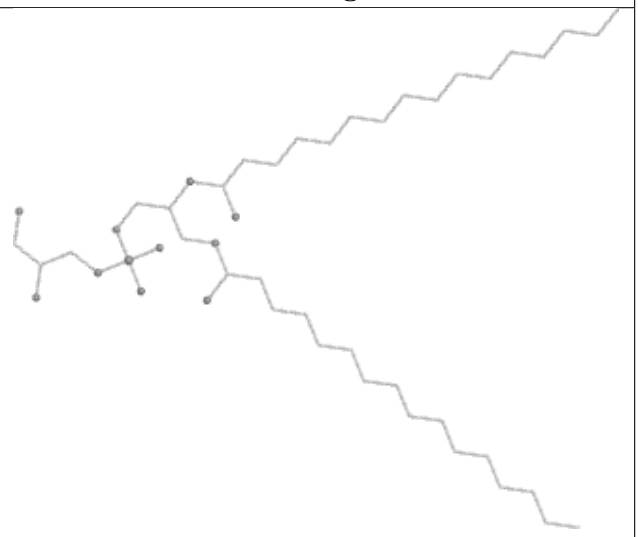
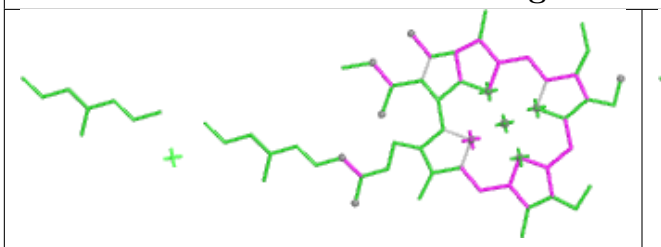


Rings

Ligand CHL 5 607



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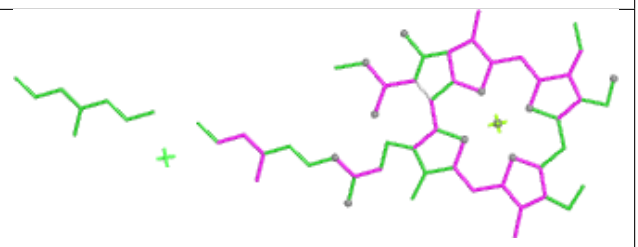
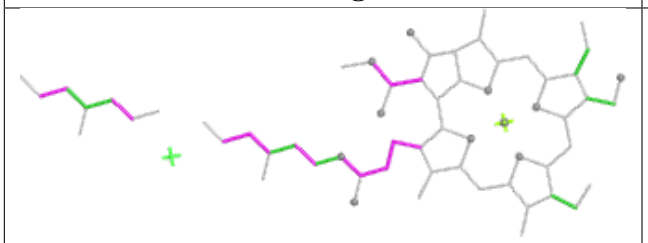


Bond angles



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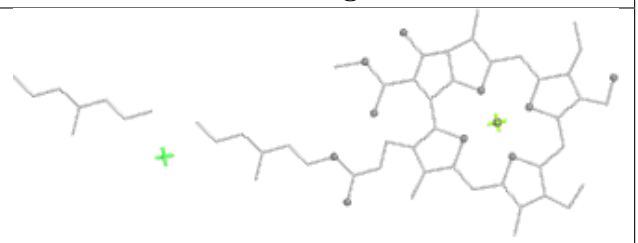
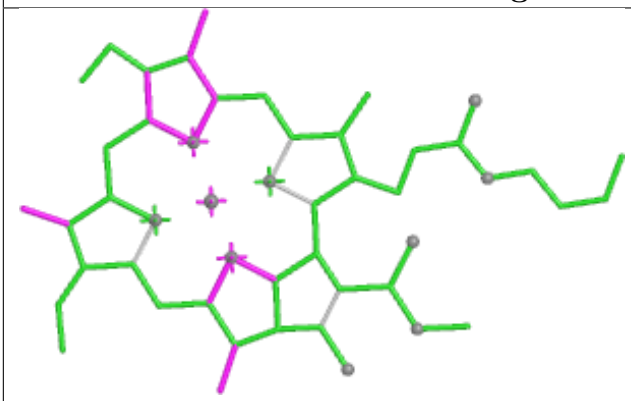


Rings

Ligand CLA BU 601



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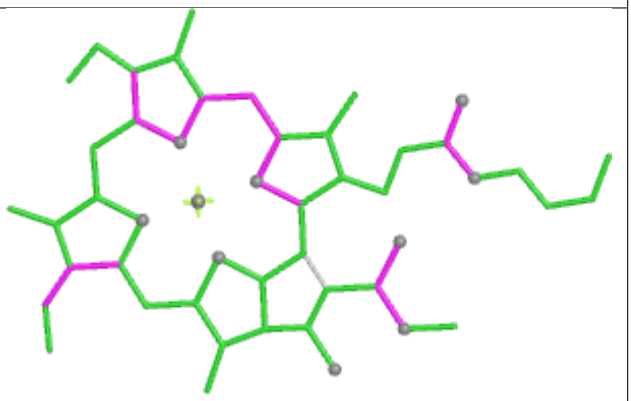

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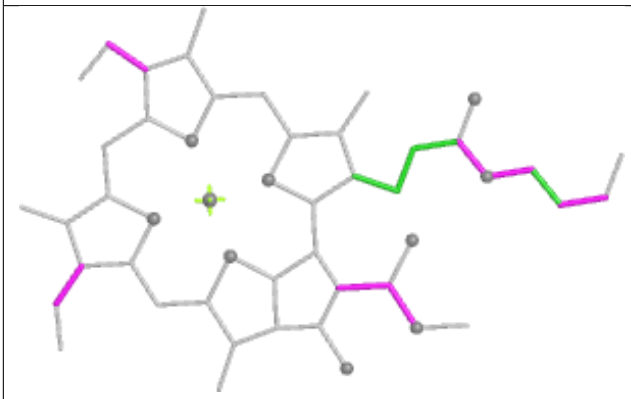

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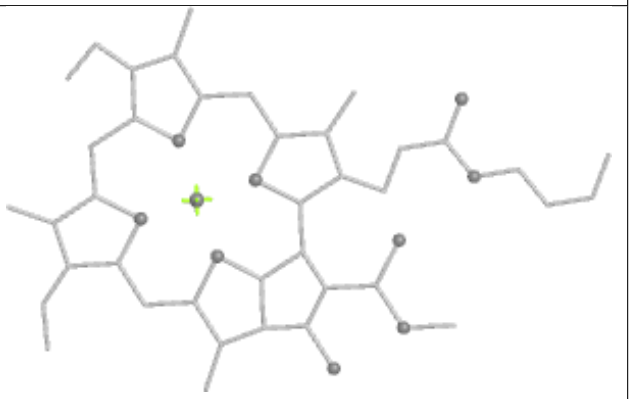

Rings

Ligand BCR B 618

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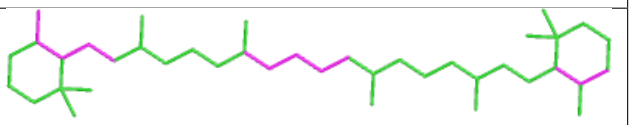

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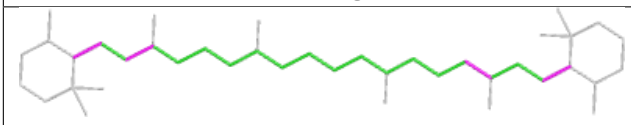

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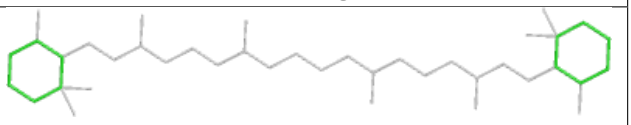
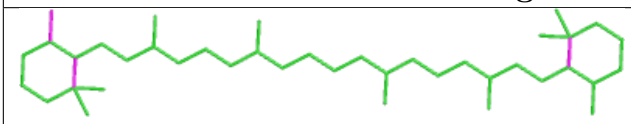


Rings

Ligand BCR BI 101



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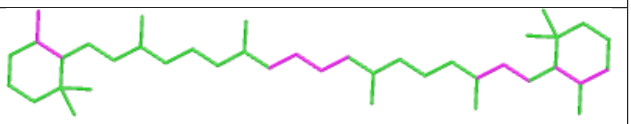
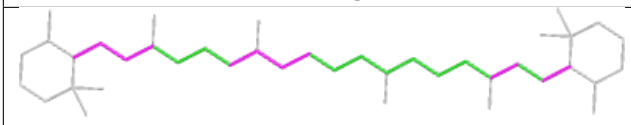


Bond angles



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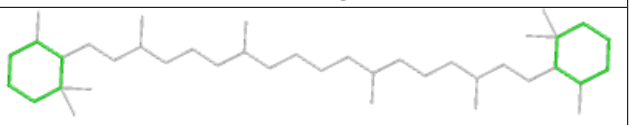
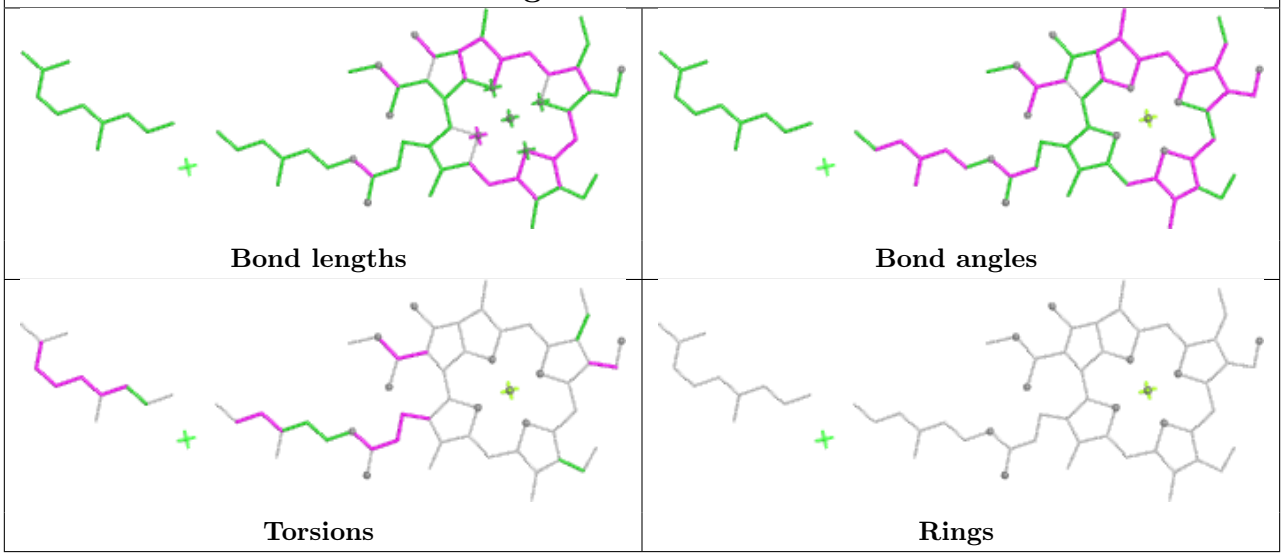


Rings

Ligand CHL G 608



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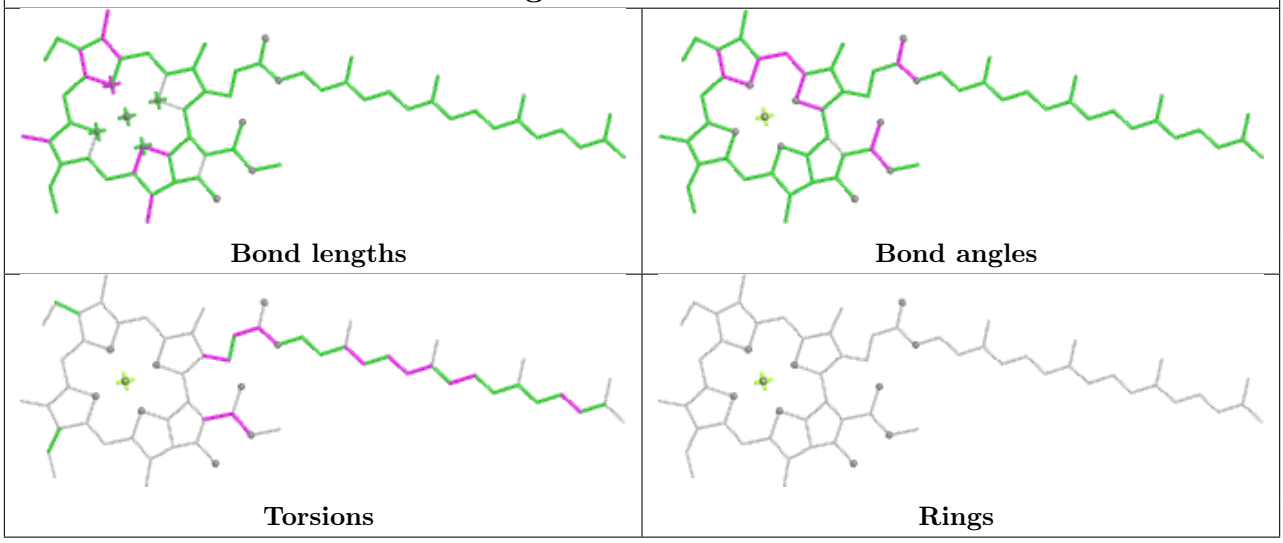

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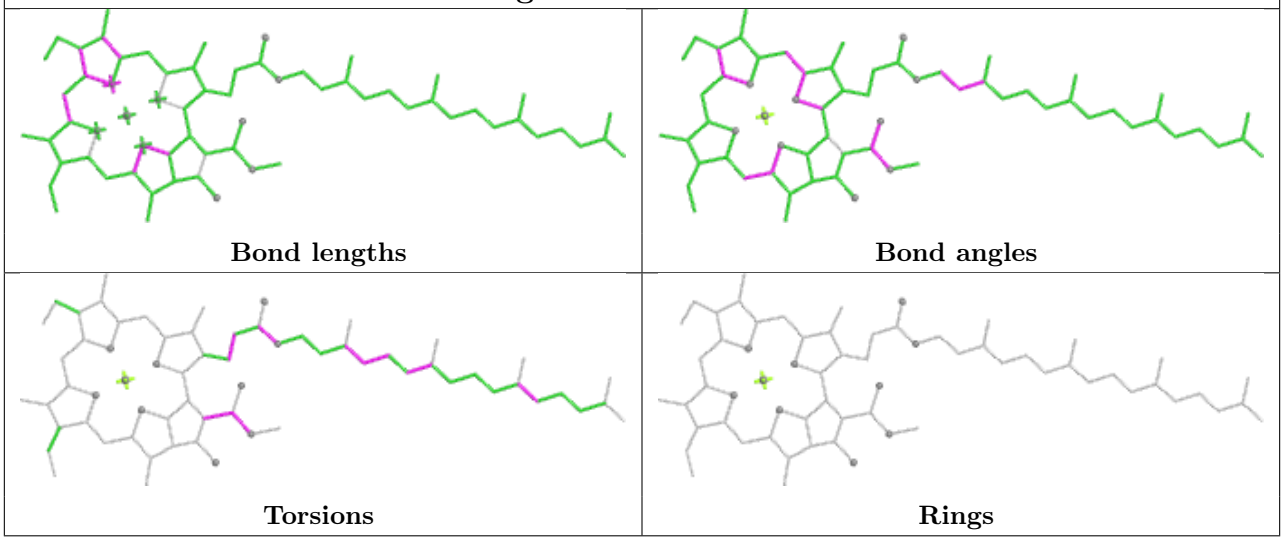
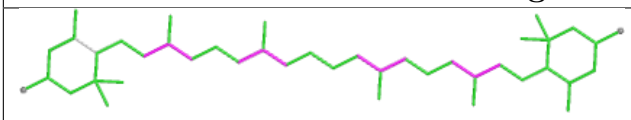
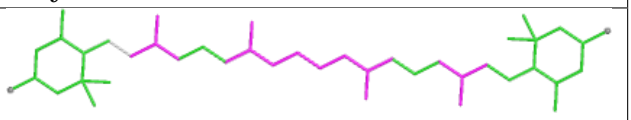
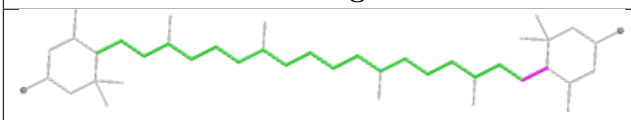
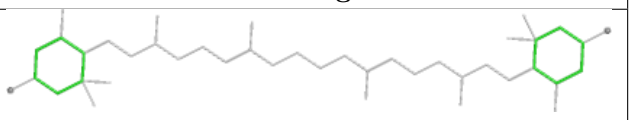
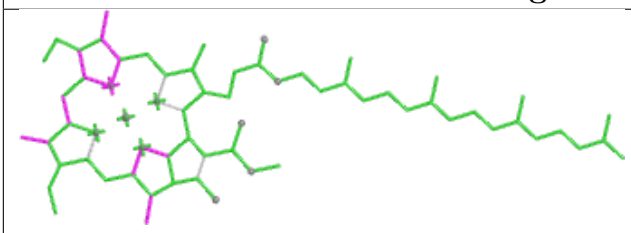
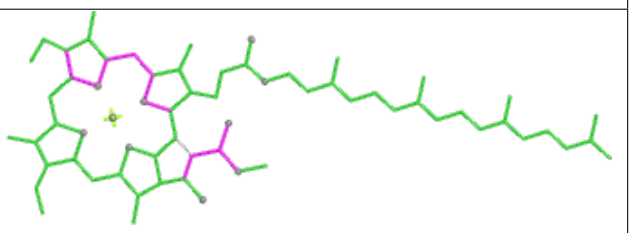
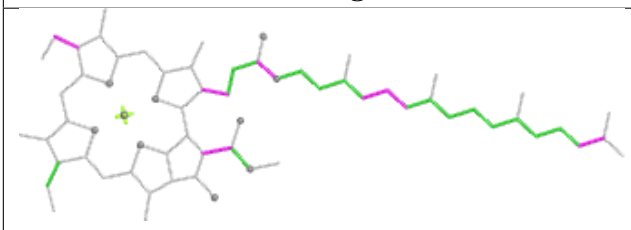
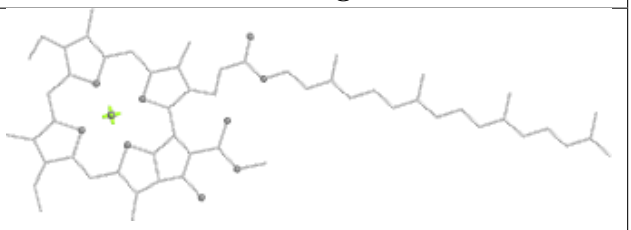


Ligand LUT y 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

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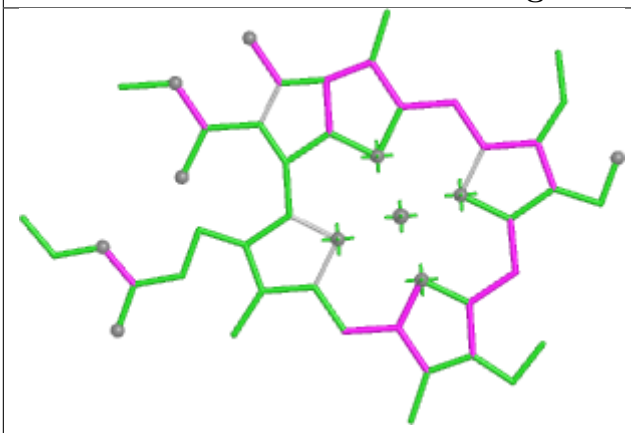
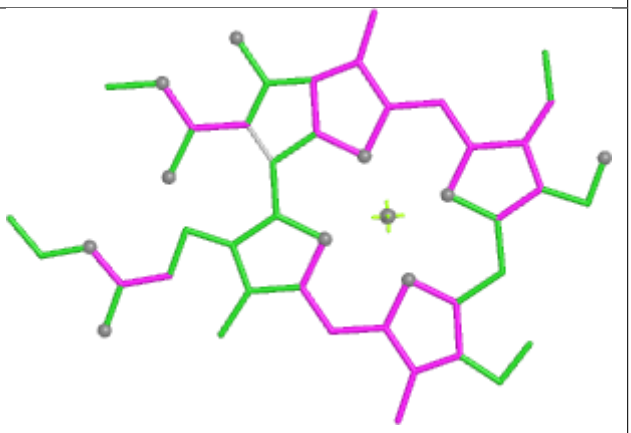
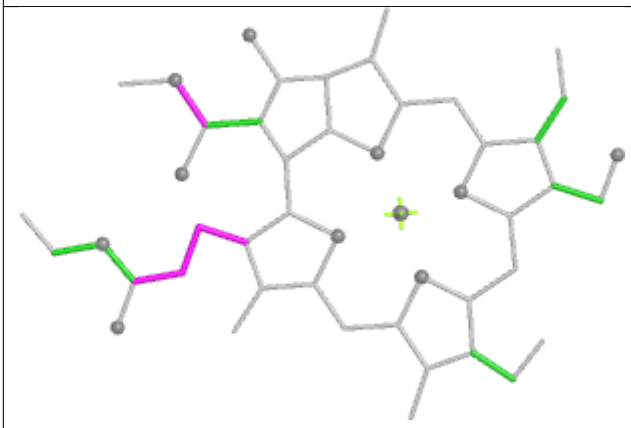
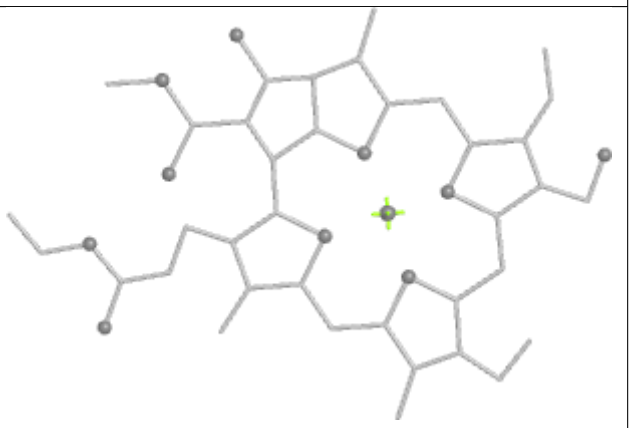
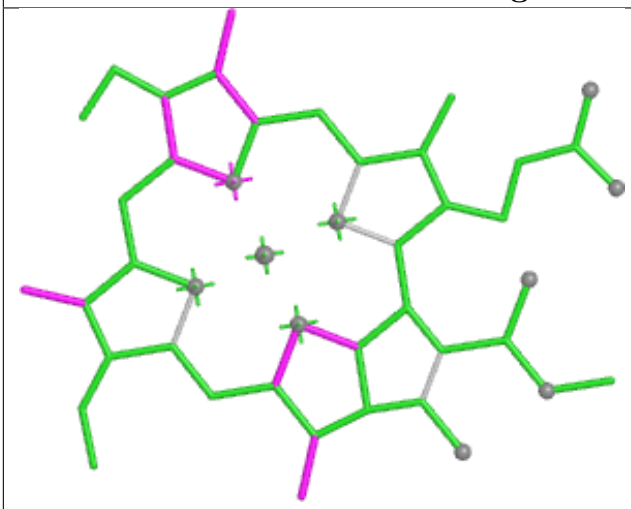
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BU 614



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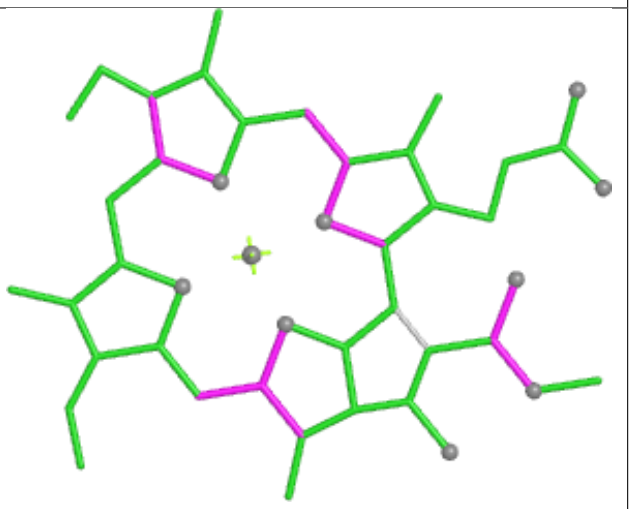

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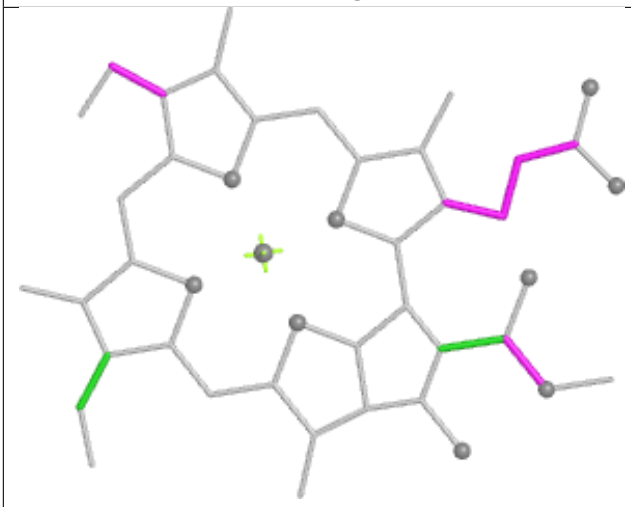
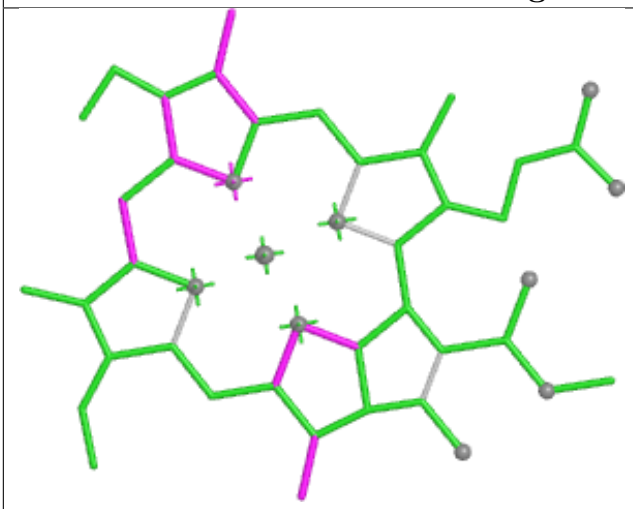


Torsions

Rings

Ligand CLA 7 315



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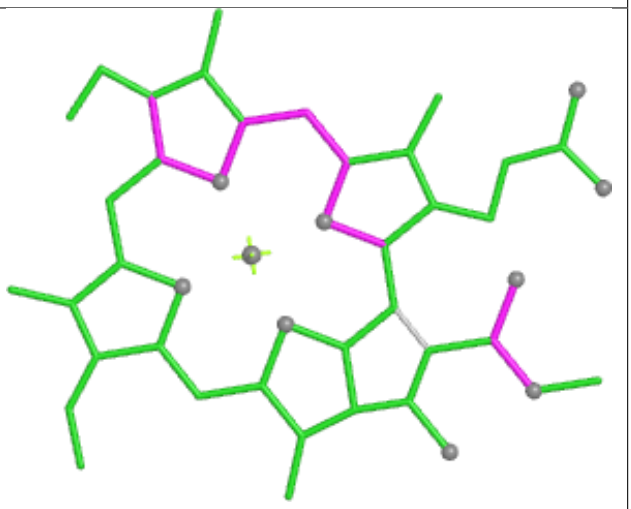

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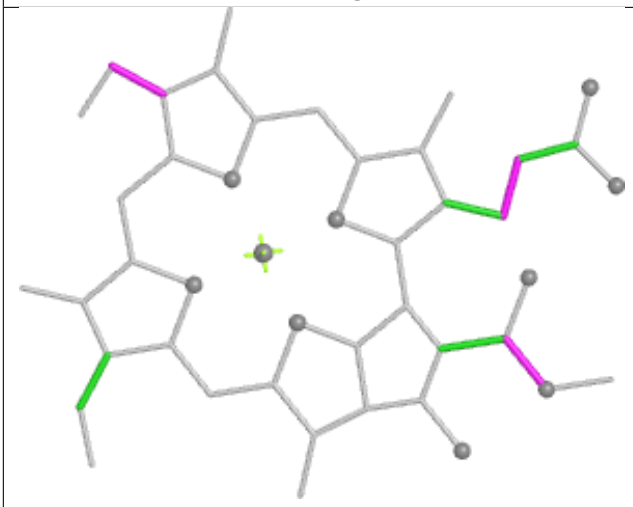
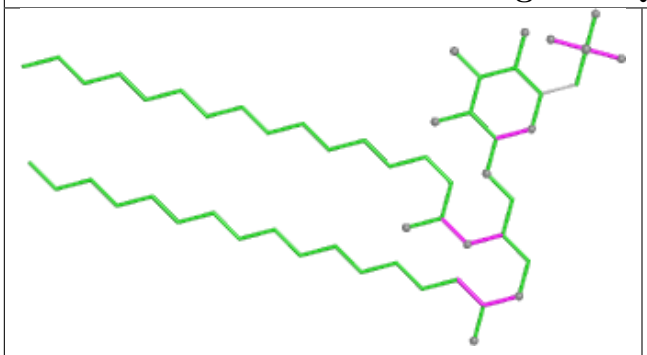


Torsions

Rings

Ligand SQD A1 101



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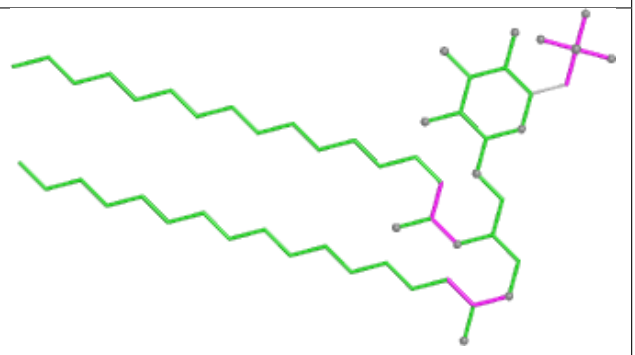

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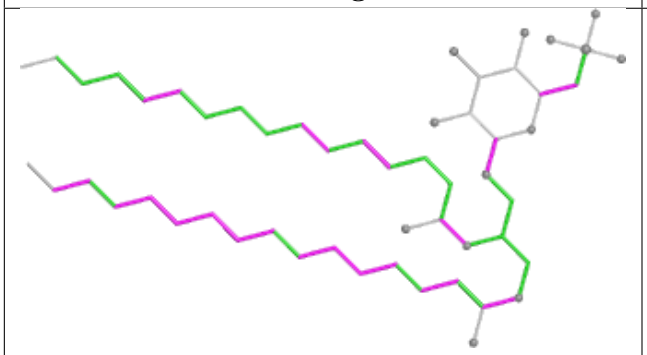

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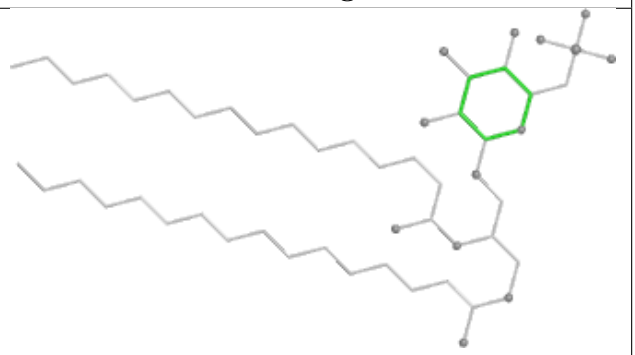
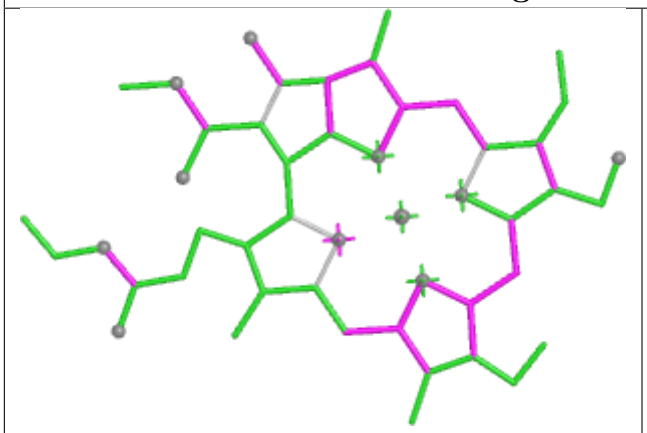


Rings

Ligand CHL BB 306



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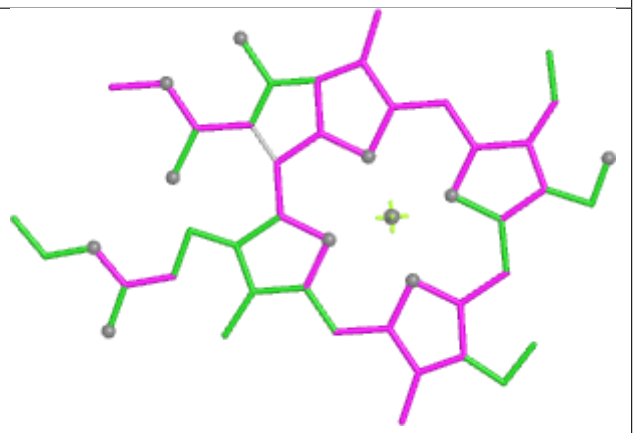
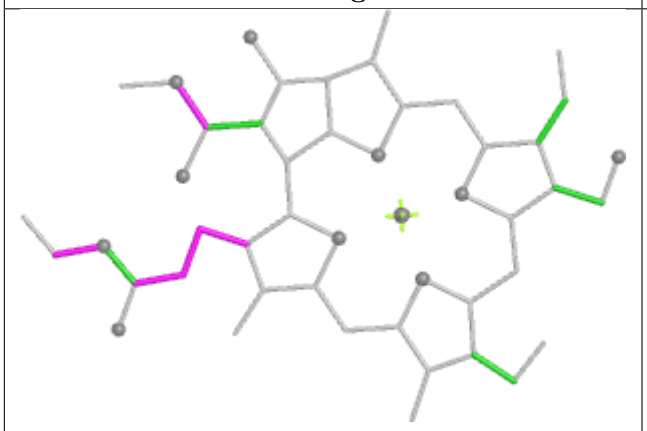


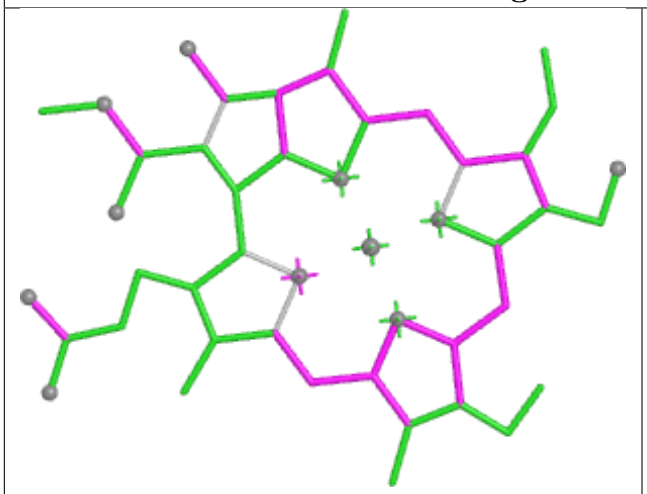
Bond angles



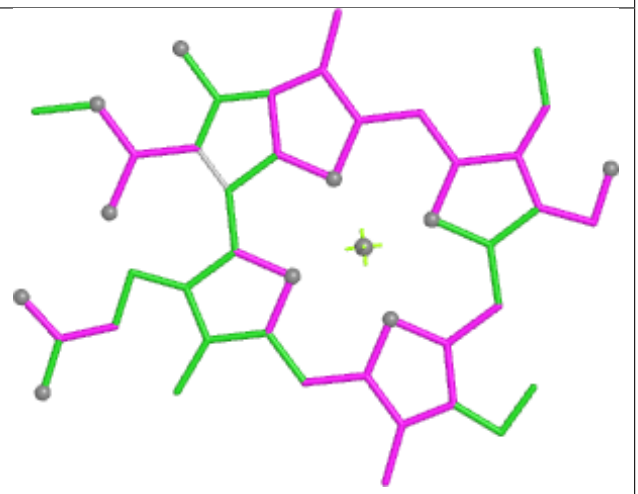
Torsions

Rings

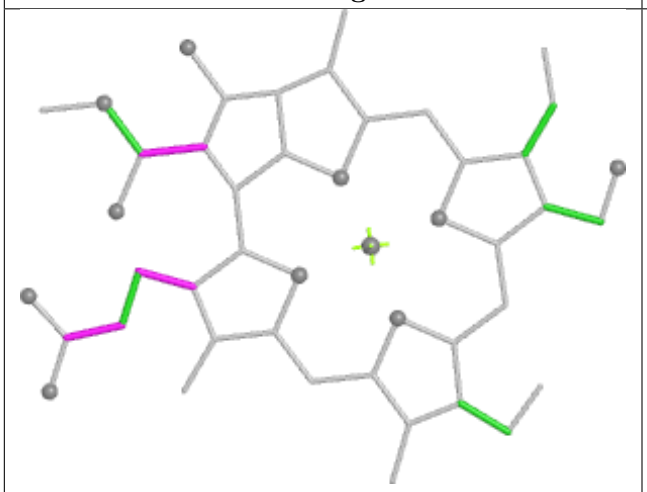
Ligand CHL AA 302



Bond lengths



Bond angles



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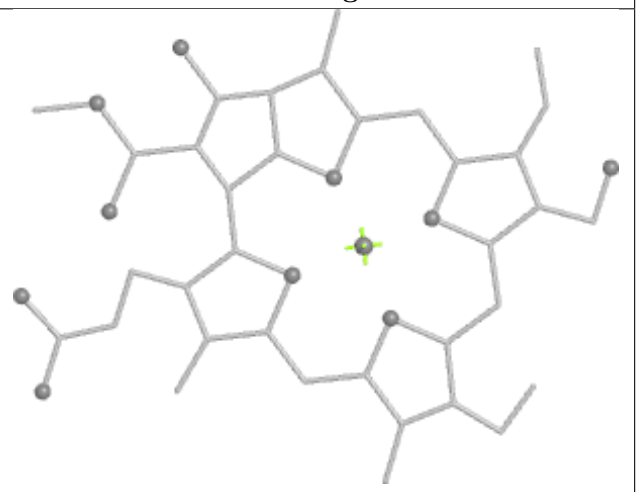
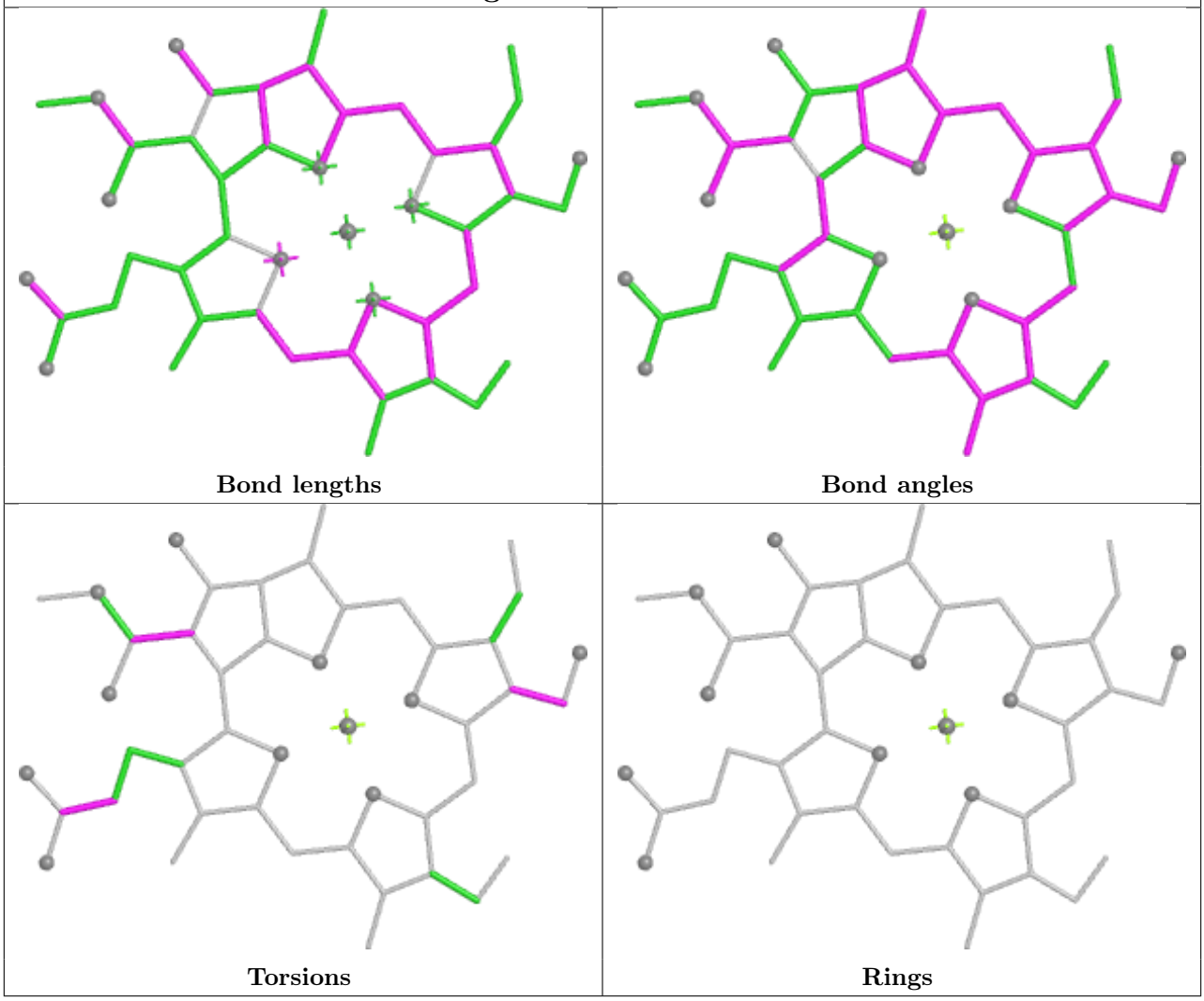
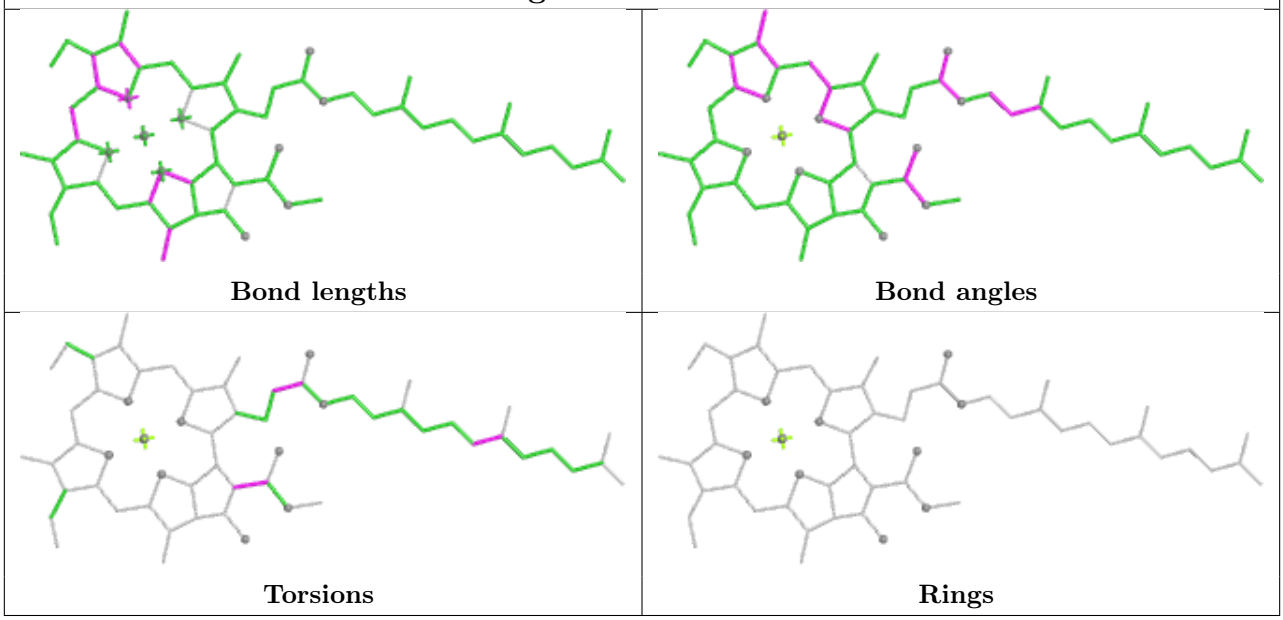


Rings

Ligand CHL A6 601



Ligand CLA n 612



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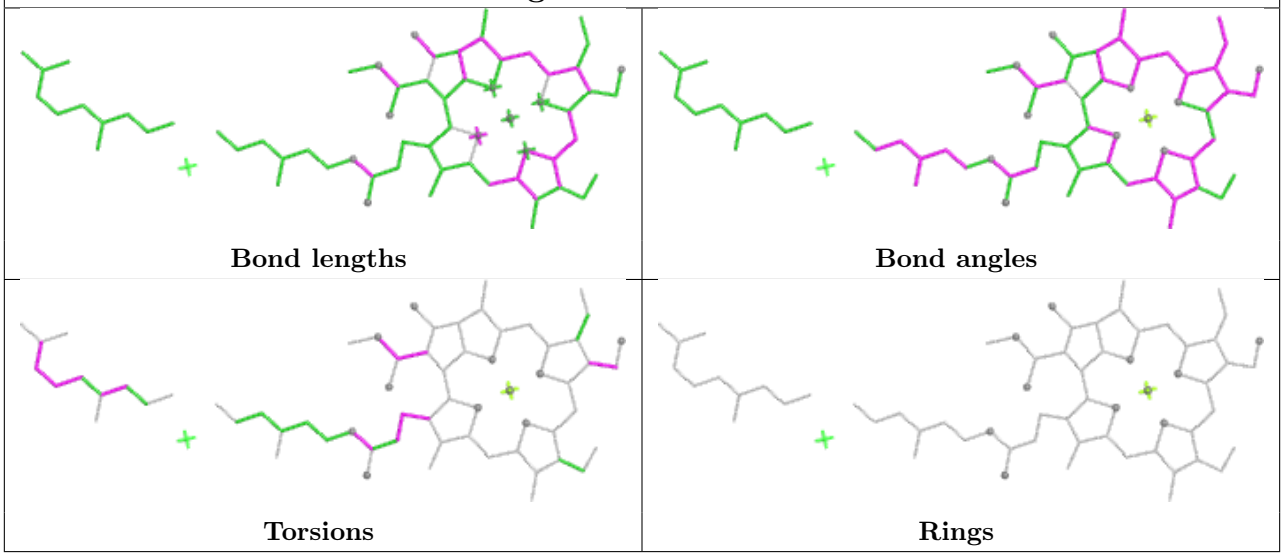
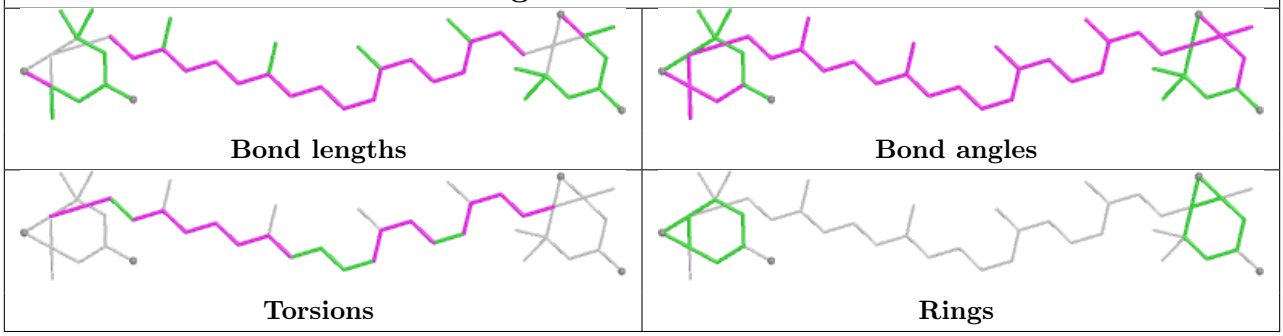


Ligand XAT AB 312



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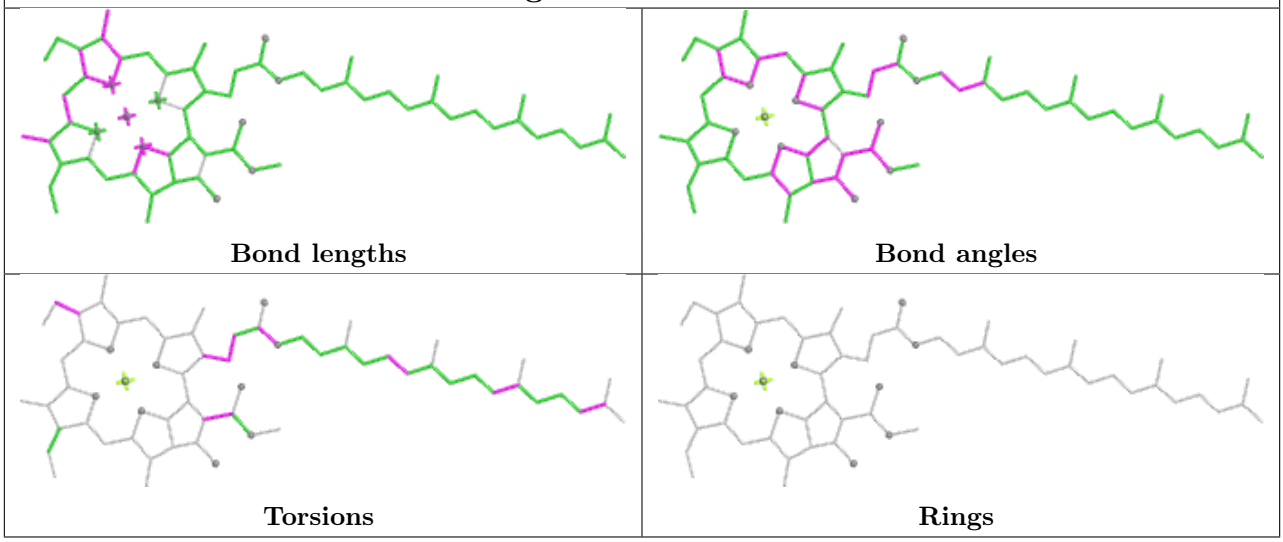
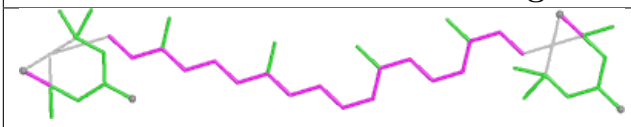
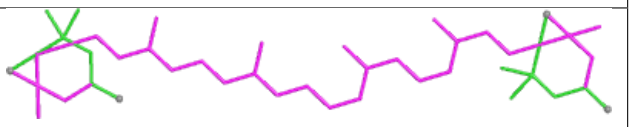
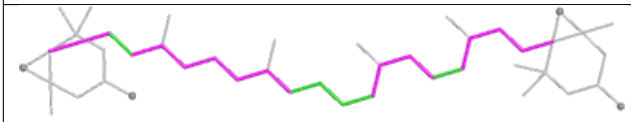
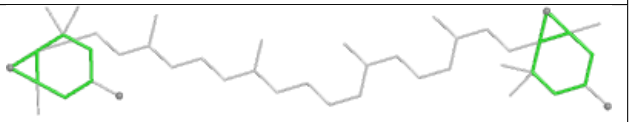


Ligand XAT 8 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

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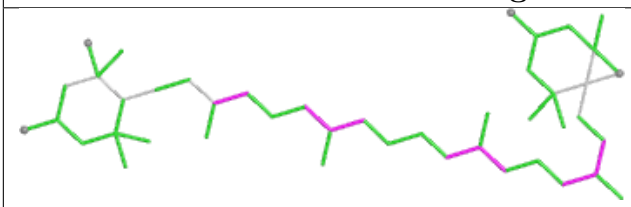
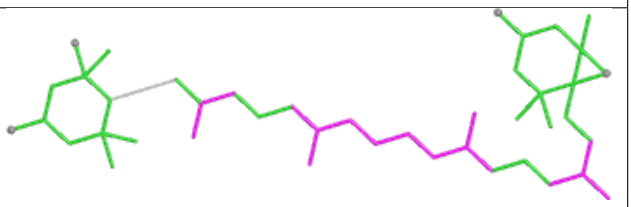
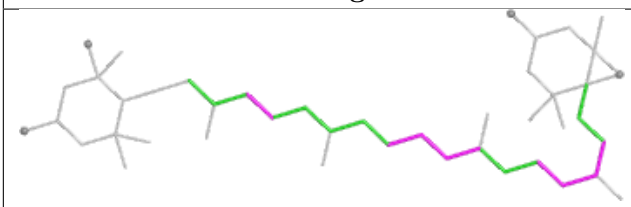
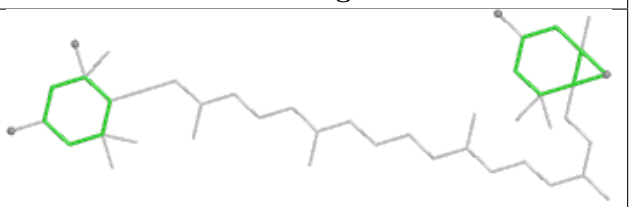
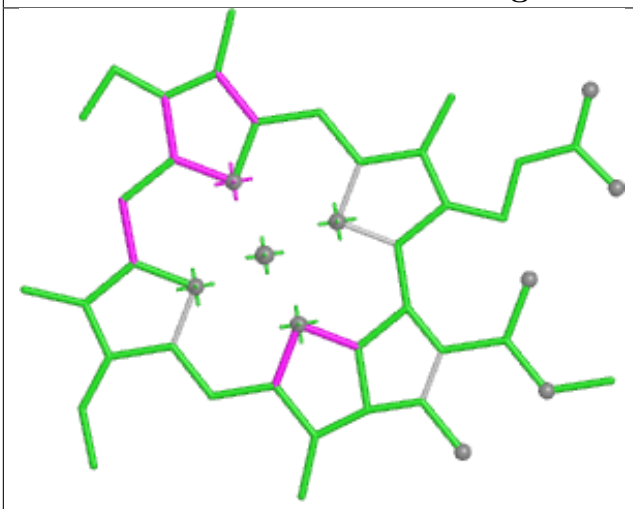
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AB 309



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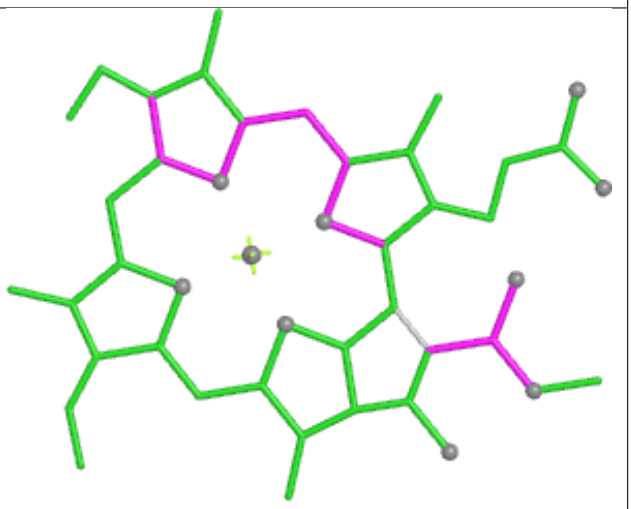

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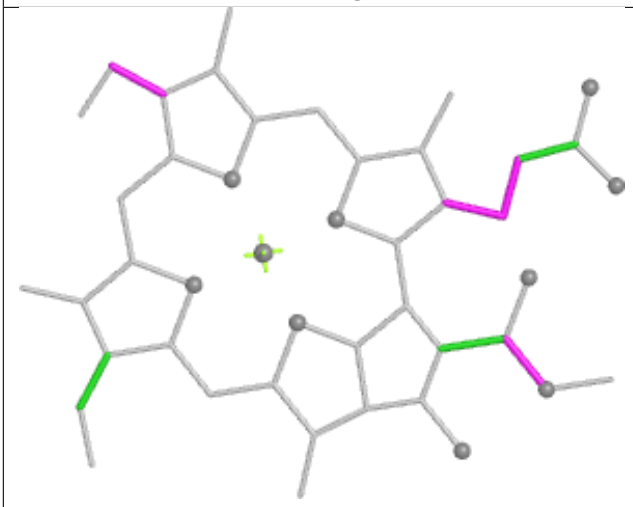
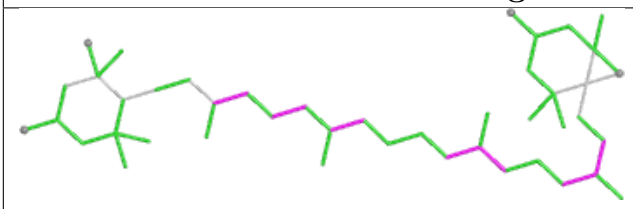


Torsions

Rings

Ligand NEX AA 319



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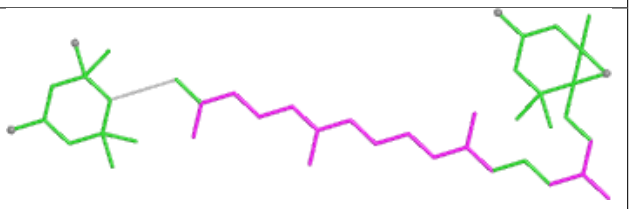

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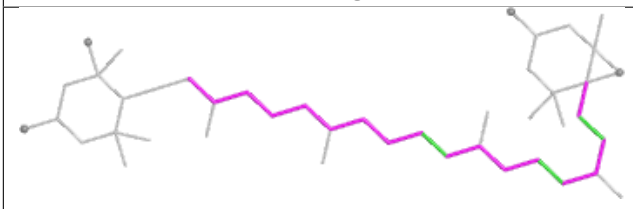

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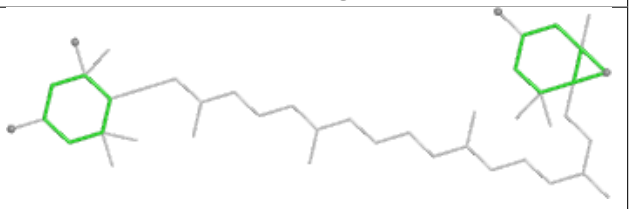
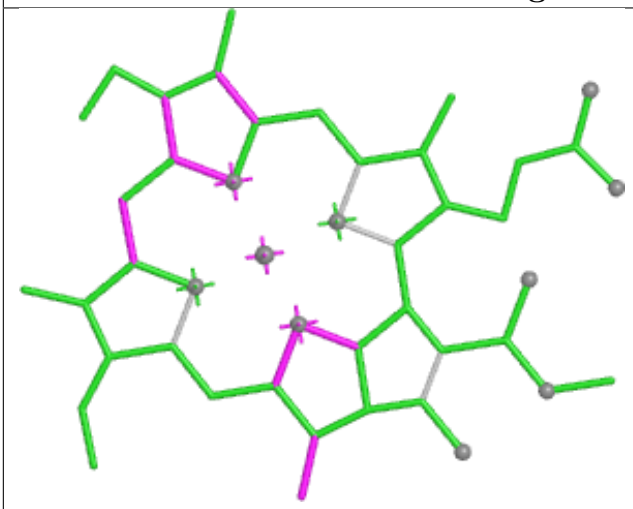


Rings

Ligand CLA 8 309



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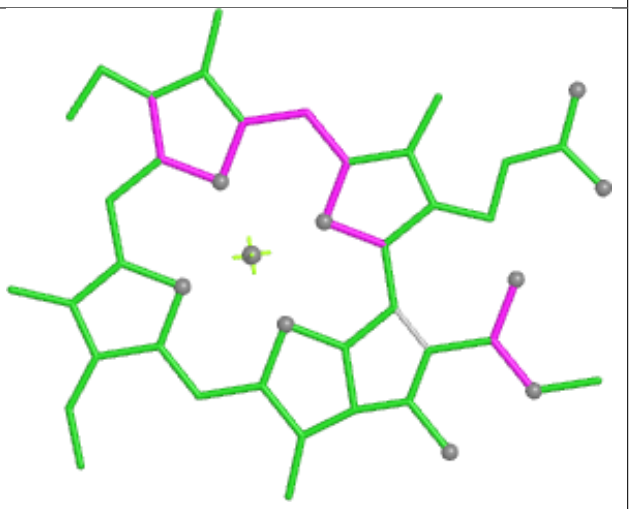

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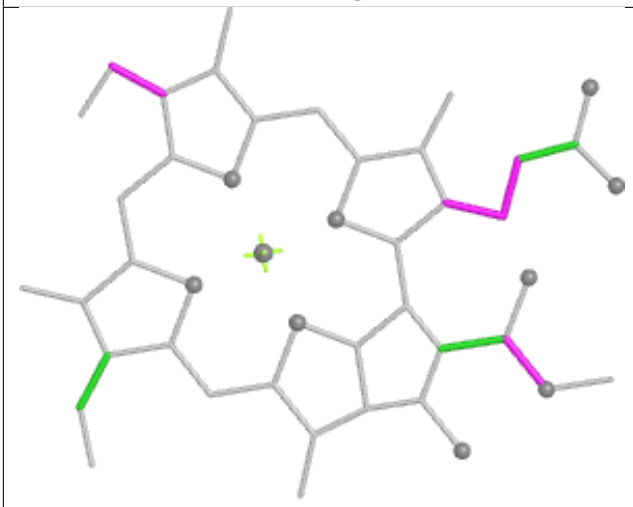
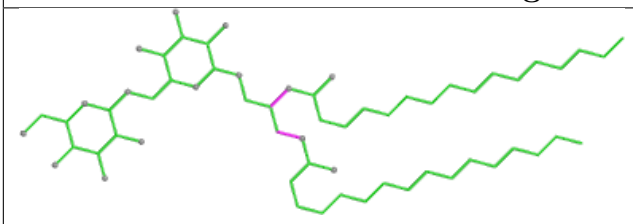


Torsions

Rings

Ligand DGD h 102



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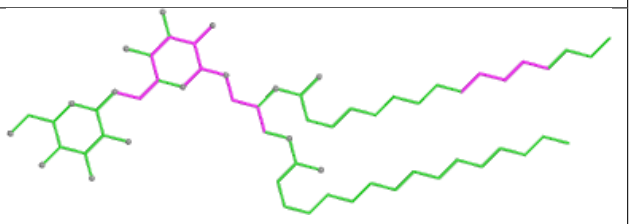

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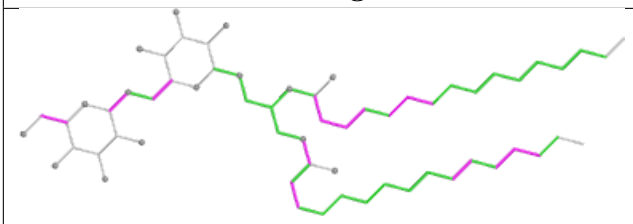

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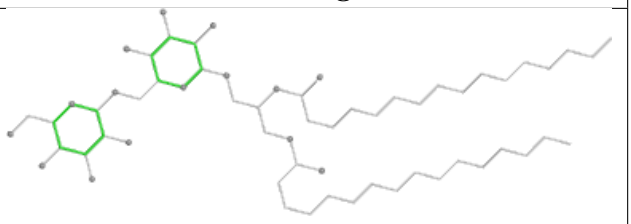
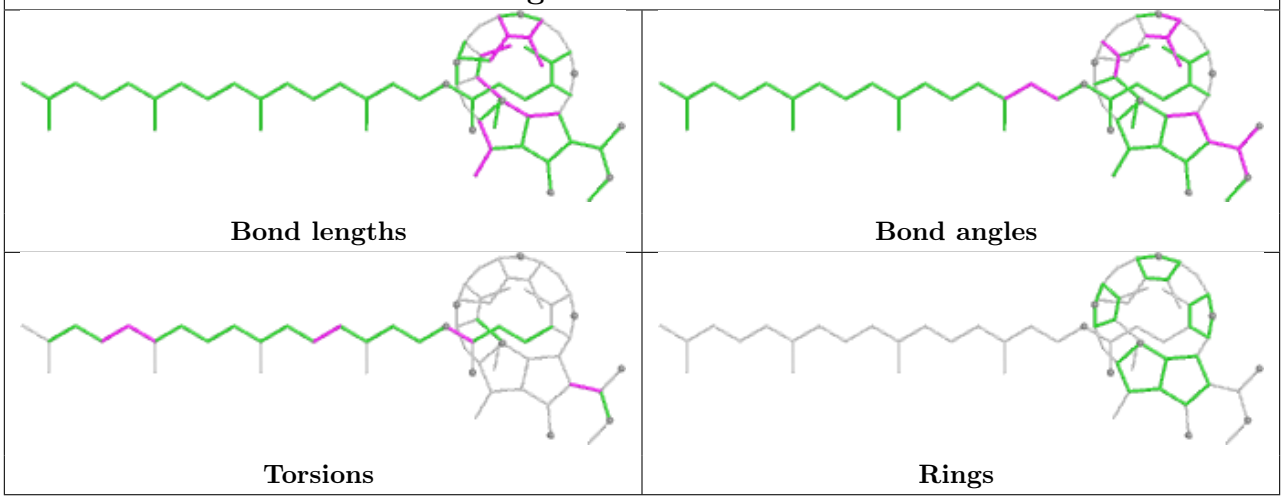
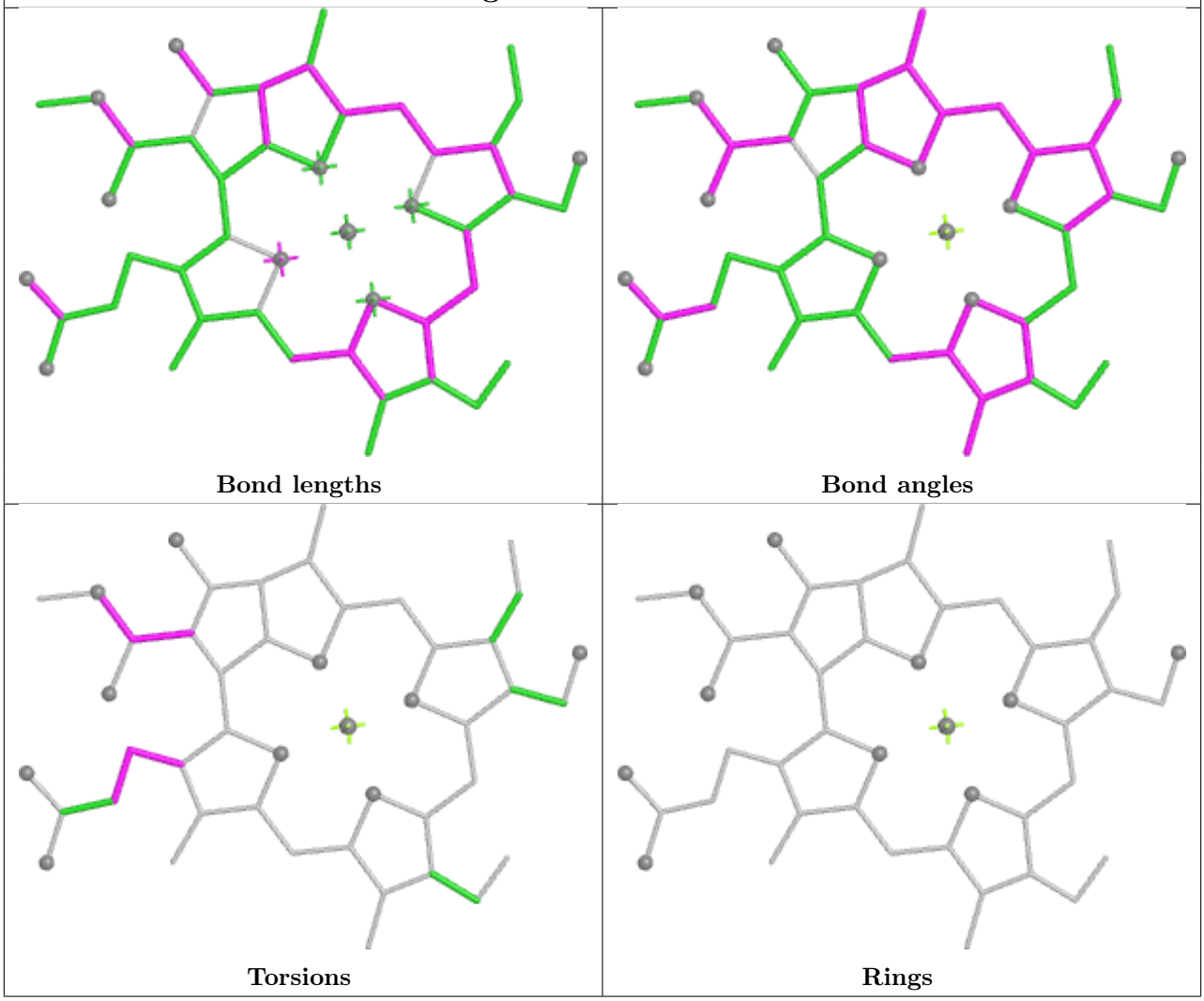


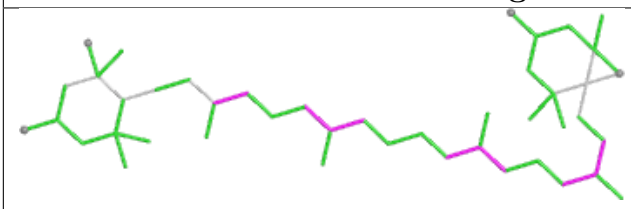
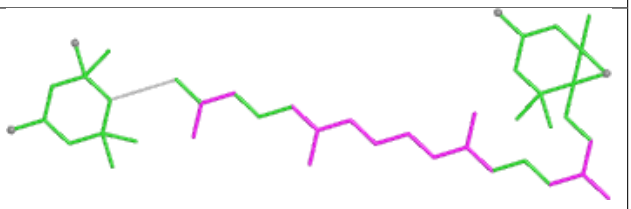
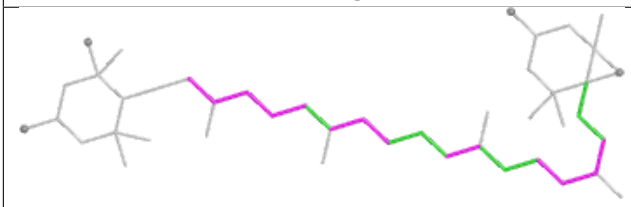
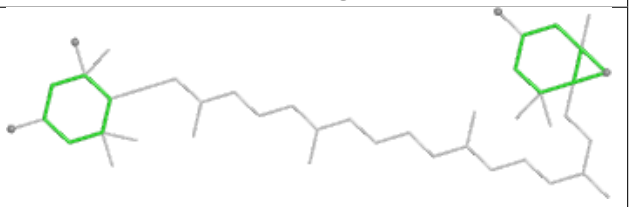
Rings

Ligand PHO a 408



Ligand CHL Au 605



Ligand NEX BV 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

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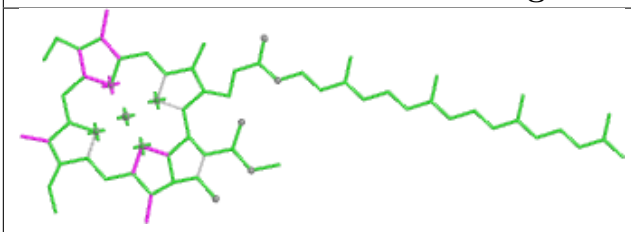
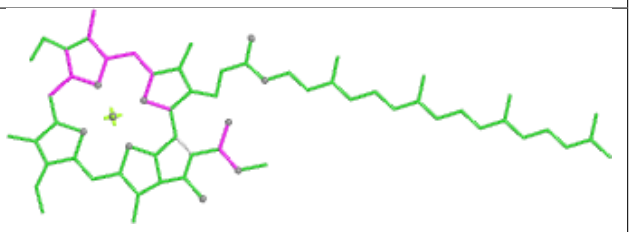
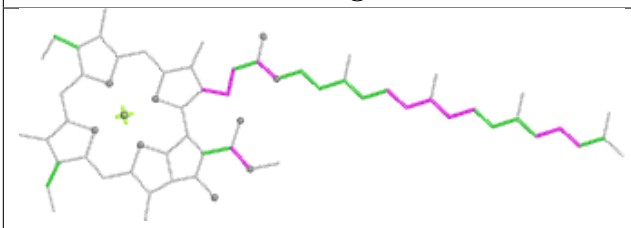
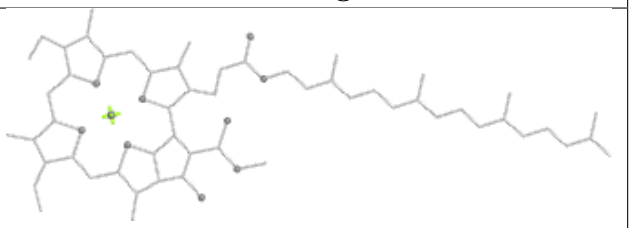
 Bond lengths	 Bond angles
 Torsions	 Rings

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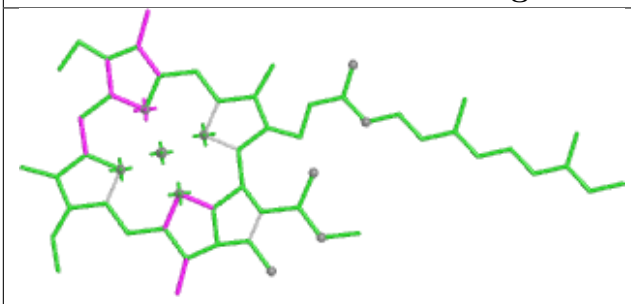
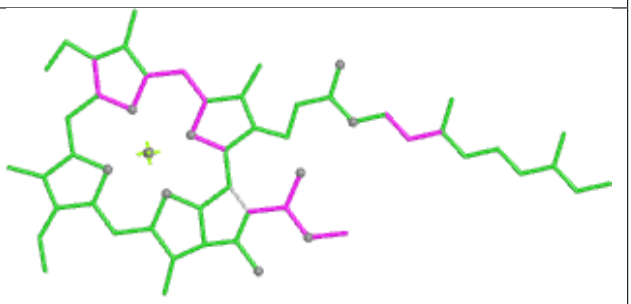
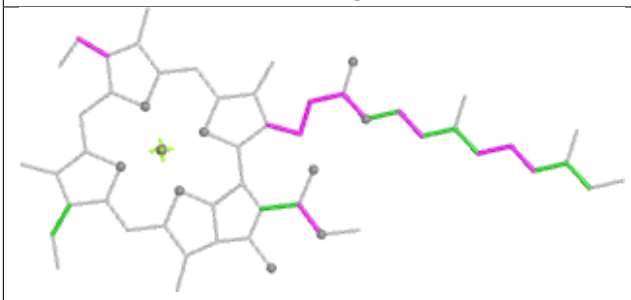
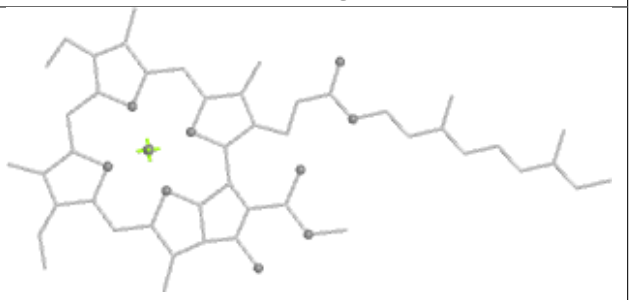
 Bond lengths	 Bond angles
 Torsions	 Rings

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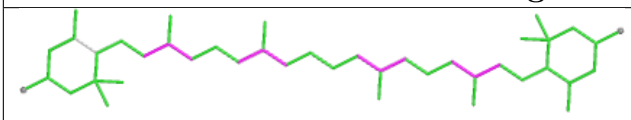
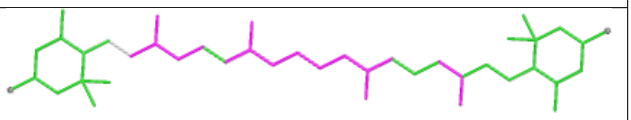
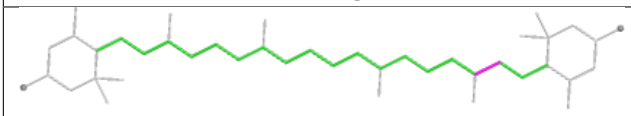
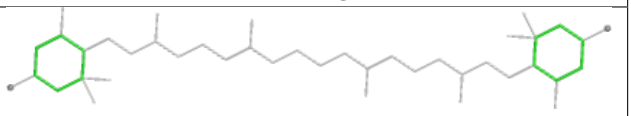
 Bond lengths	 Bond angles
 Torsions	 Rings

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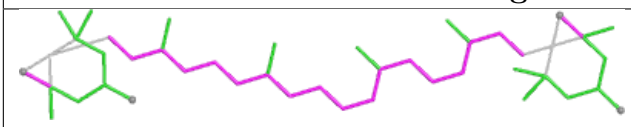
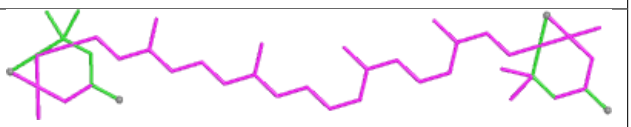
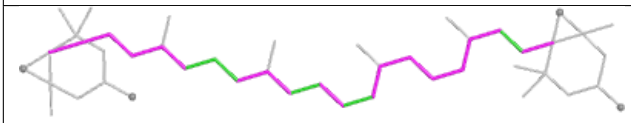
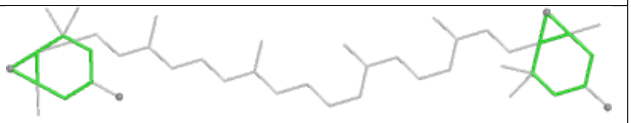
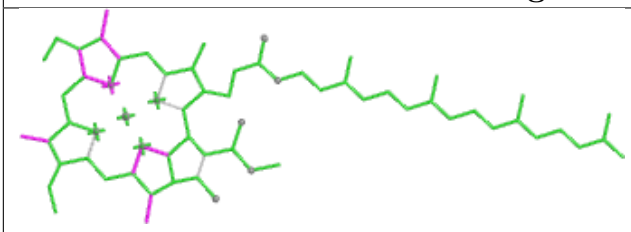
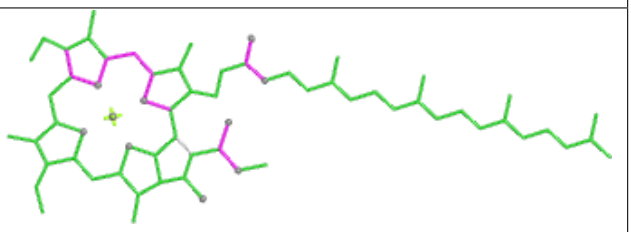
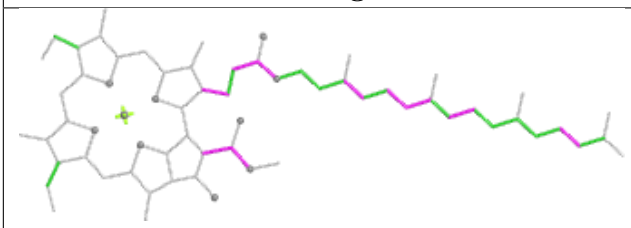
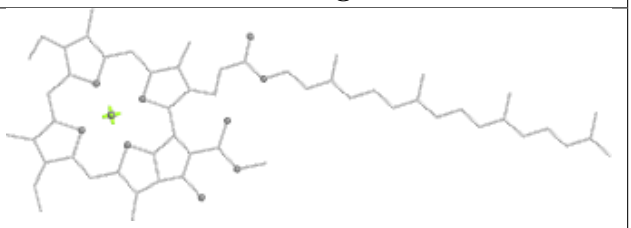
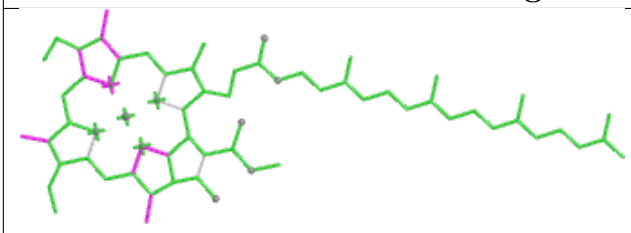
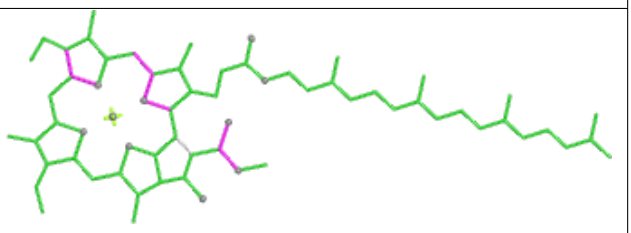
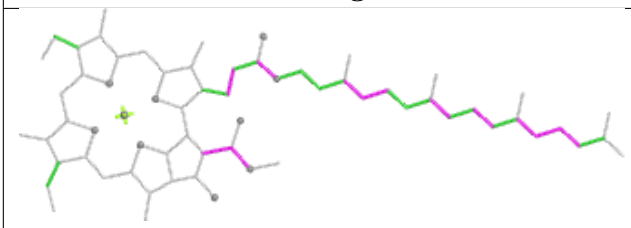
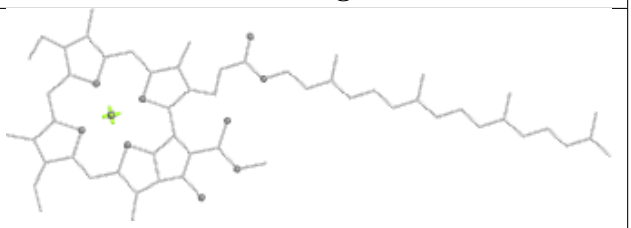
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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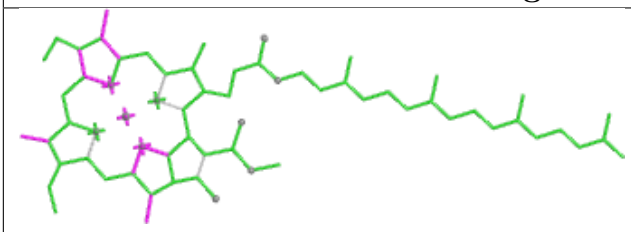
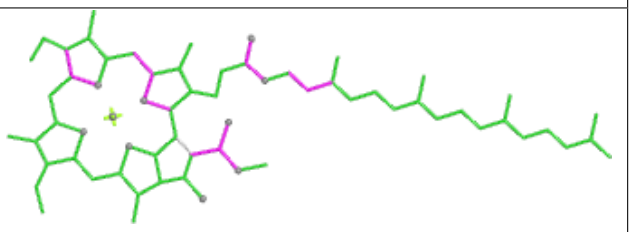
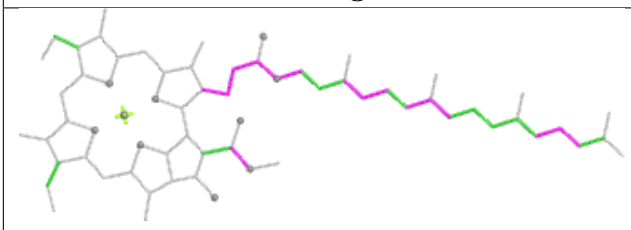
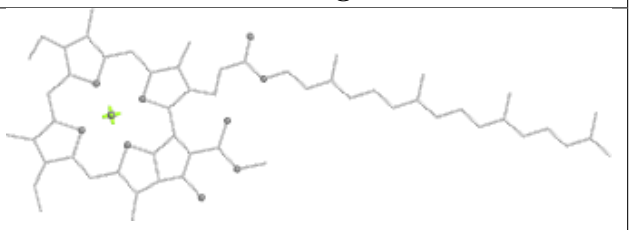
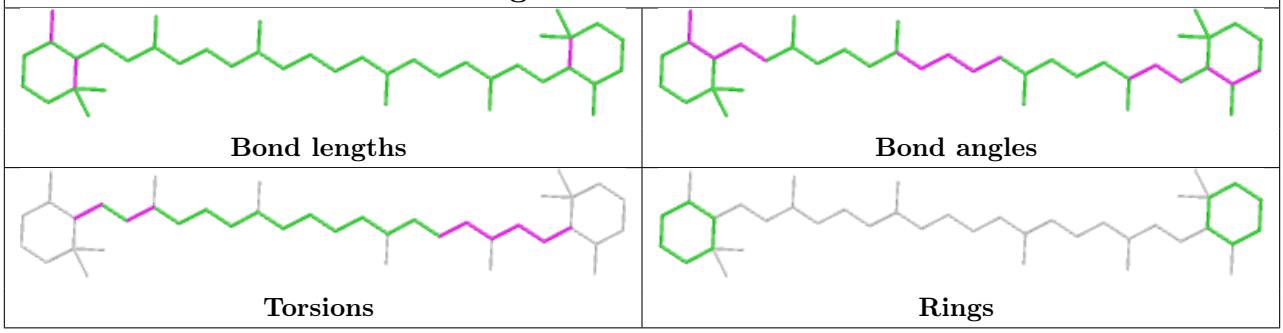
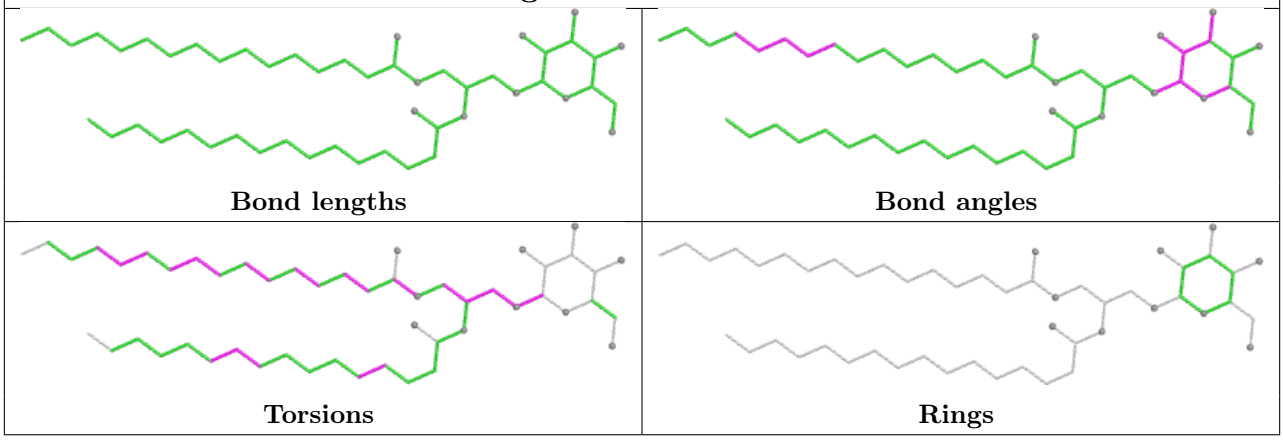
 Bond lengths	 Bond angles
 Torsions	 Rings

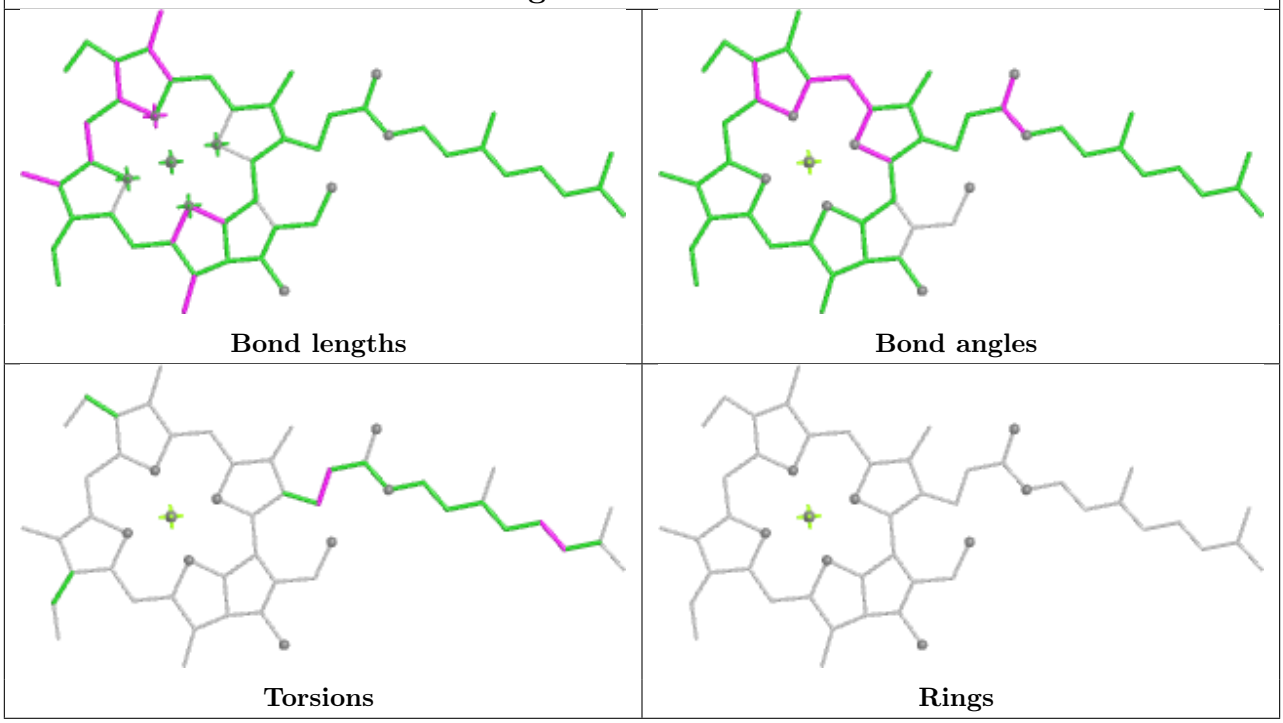
Ligand BCR BN 101



Ligand LMG C 501



Ligand CLA S 609



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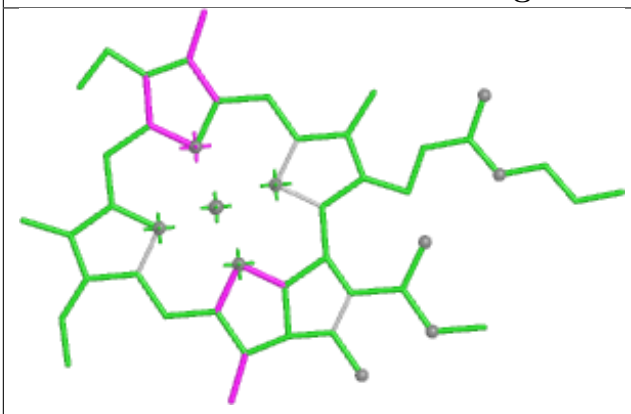
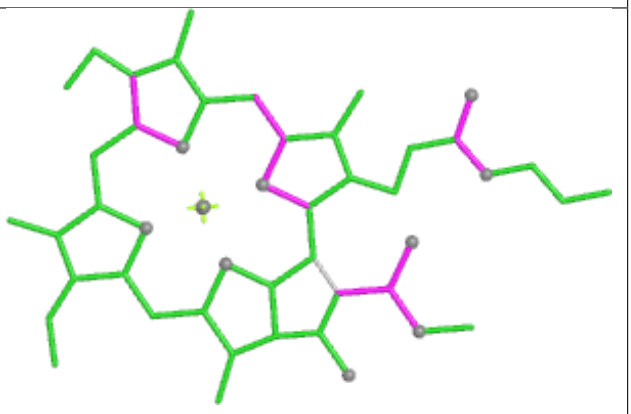
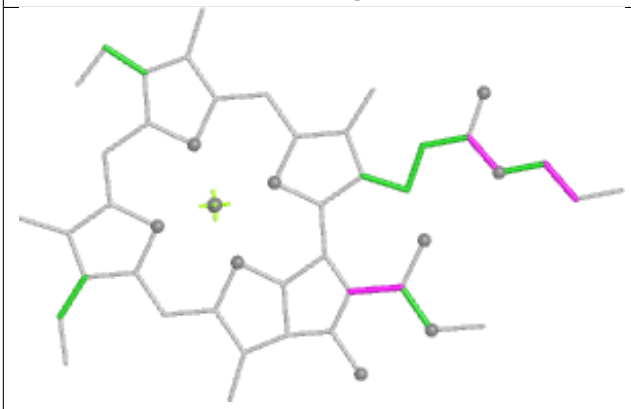


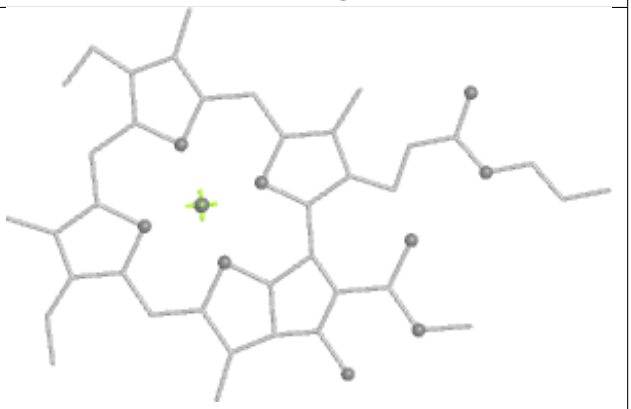
Bond lengths



Bond angles

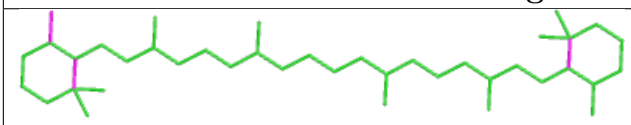


Torsions



Rings

Ligand BCR 8 313



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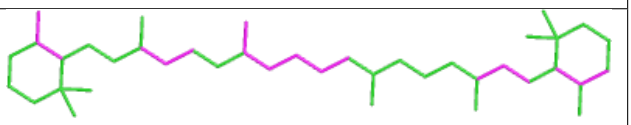
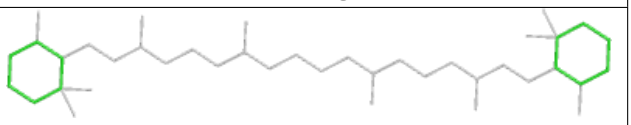
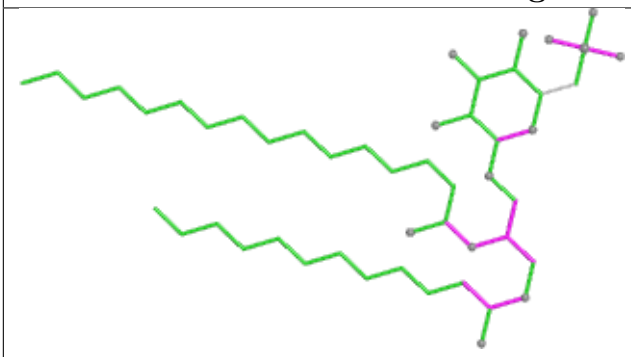
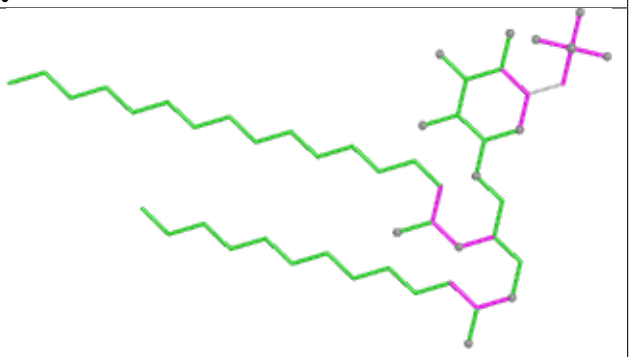
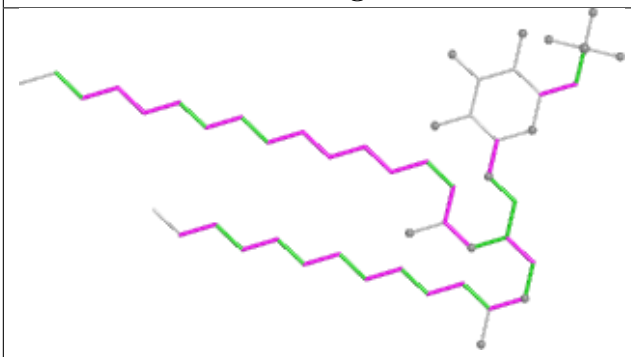
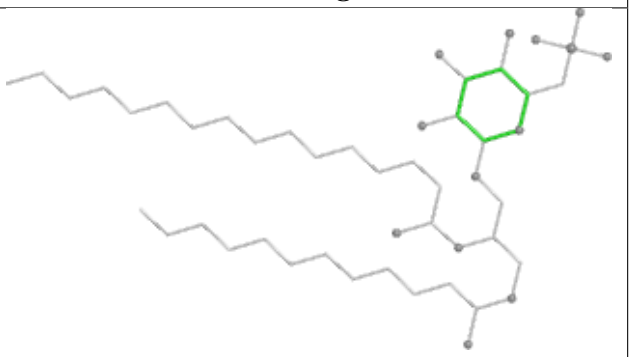


Bond angles

Torsions



Rings

Ligand SQD 2 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

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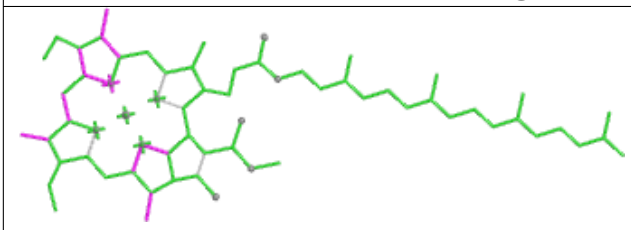
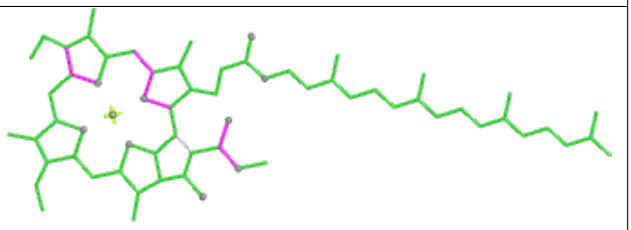
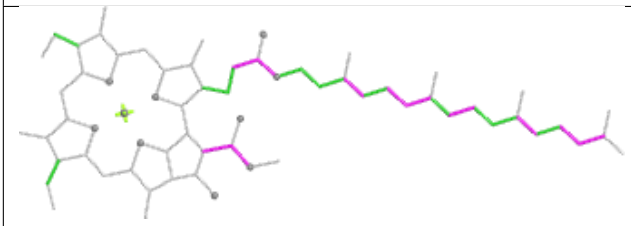
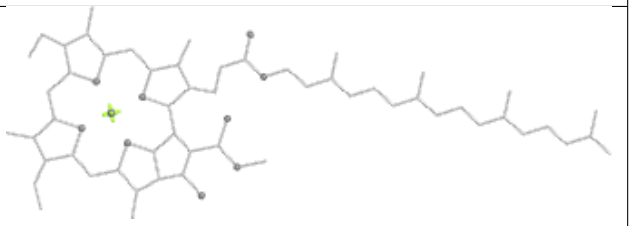
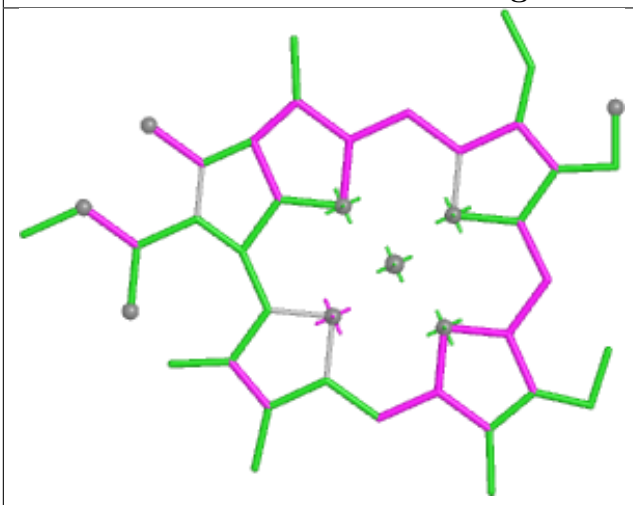
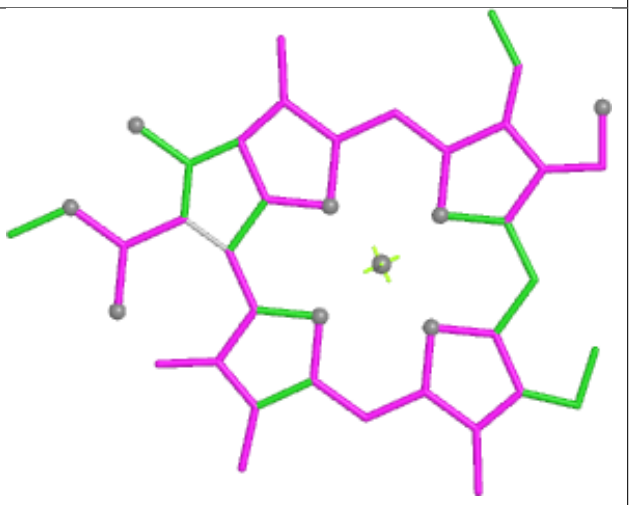
 Bond lengths	 Bond angles
 Torsions	 Rings

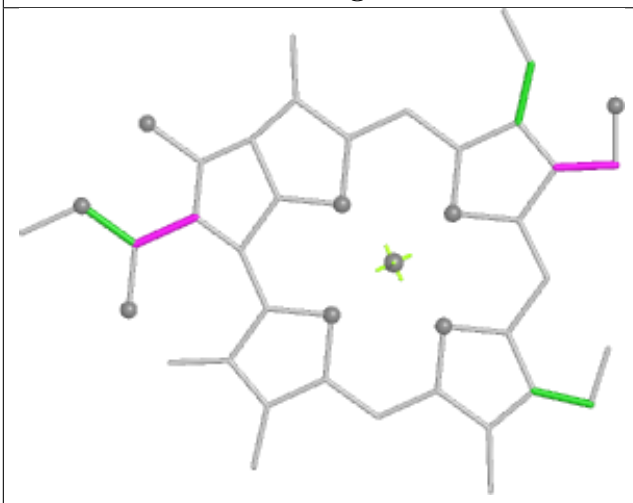
Ligand CHL BU 613



Bond lengths



Bond angles



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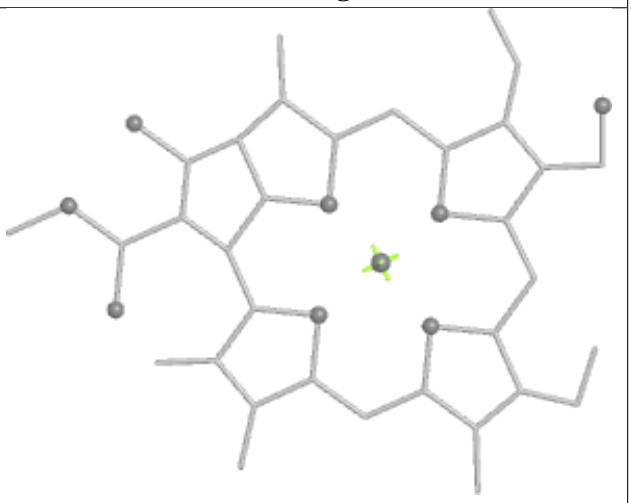
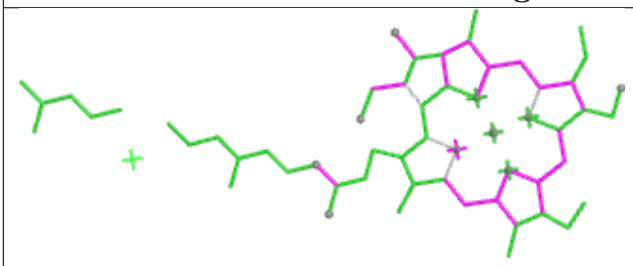


Rings

Ligand CHL Au 609



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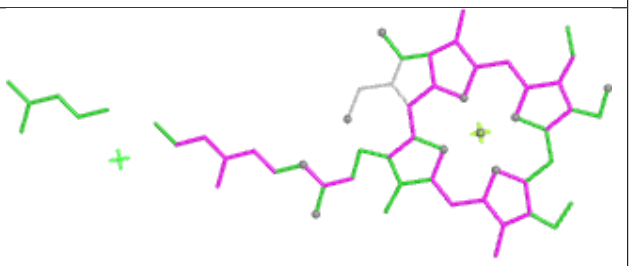
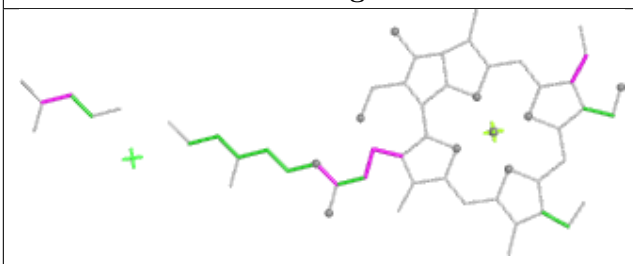


Bond angles



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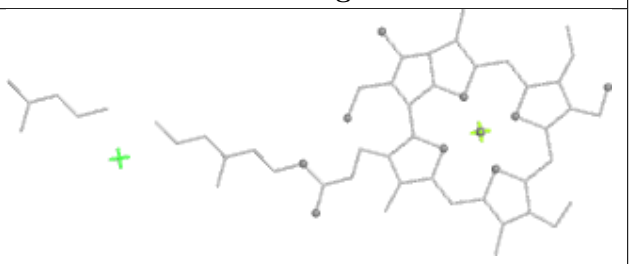
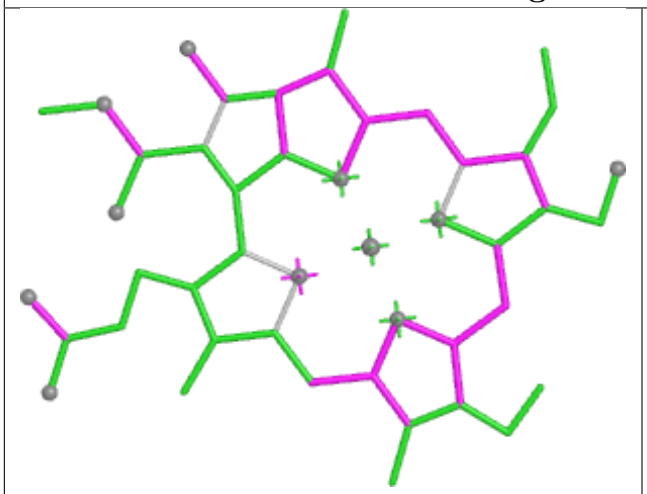
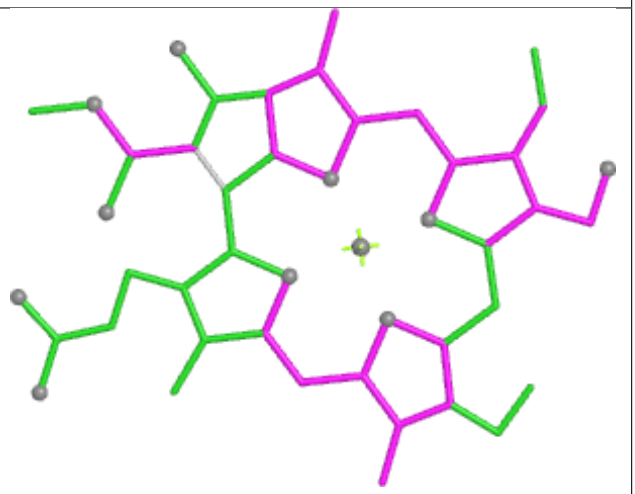


Rings

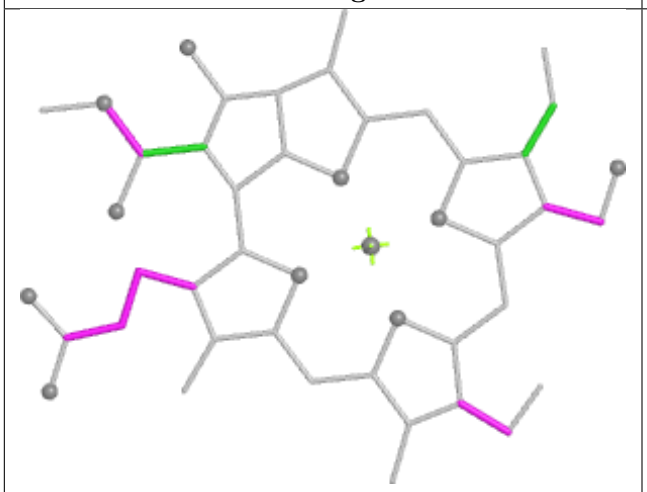
Ligand CHL 7 309



Bond lengths



Bond angles



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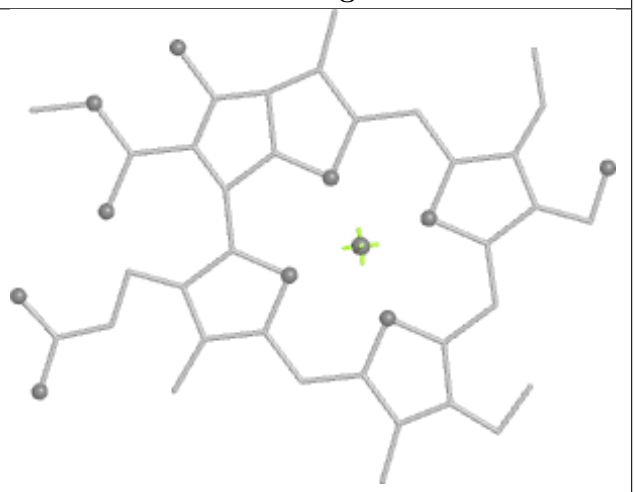
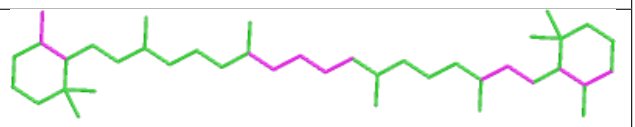


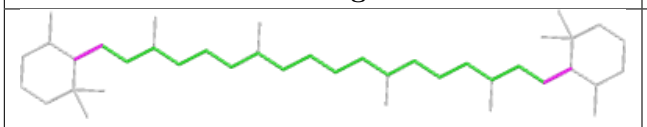
Rings

Ligand BCR C 514

Bond lengths



Bond angles



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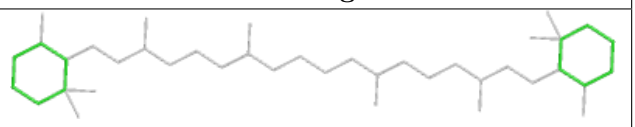
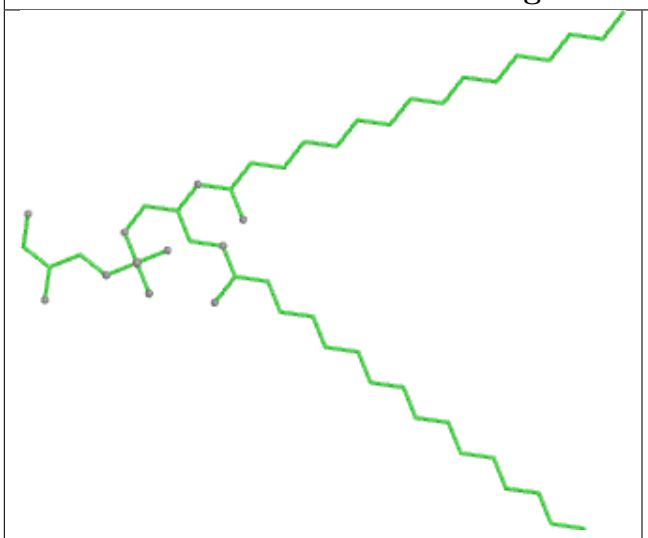
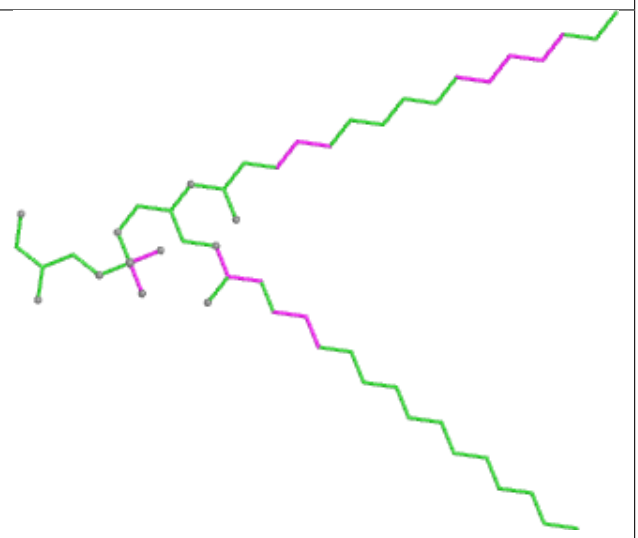


Rings

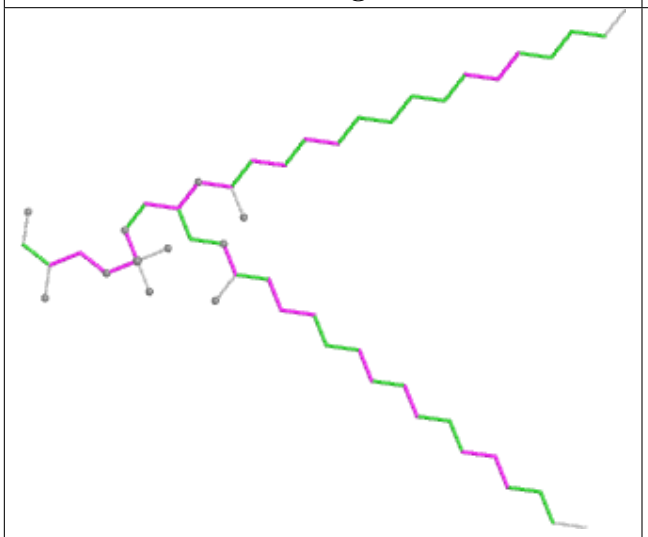
Ligand LHG C 520



Bond lengths



Bond angles



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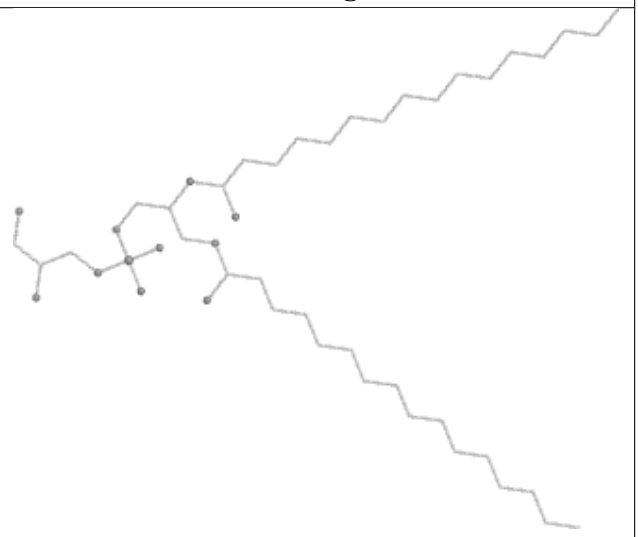
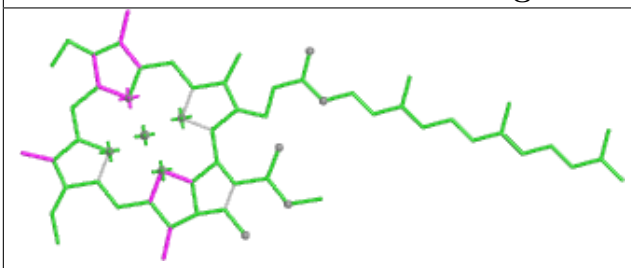
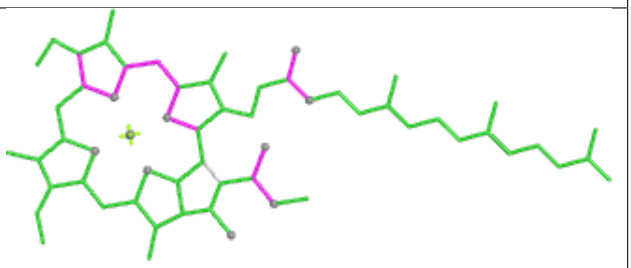


Rings

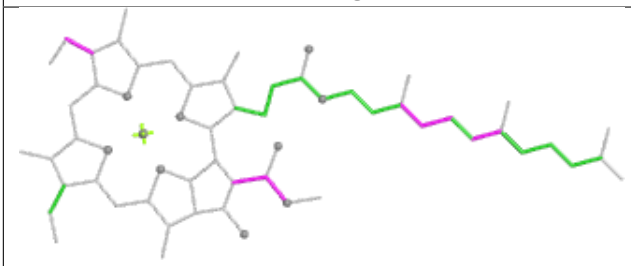
Ligand CLA Au 612



Bond lengths



Bond angles



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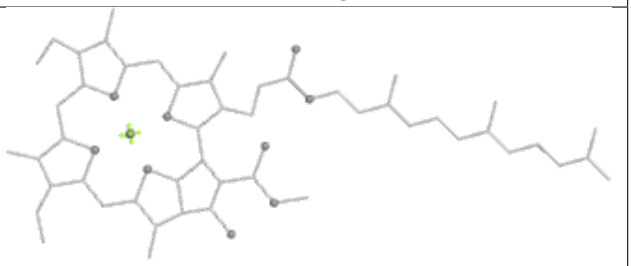
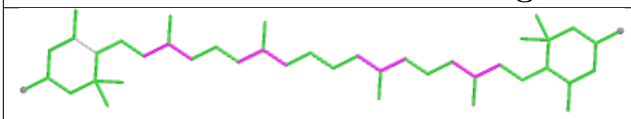


Rings

Ligand LUT Ba 317



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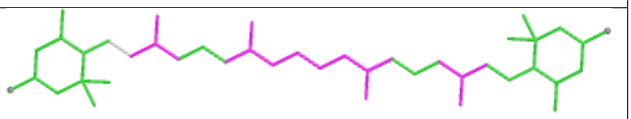
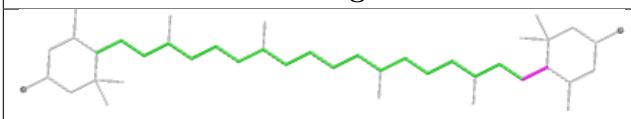


Bond angles



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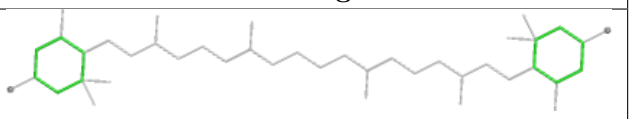
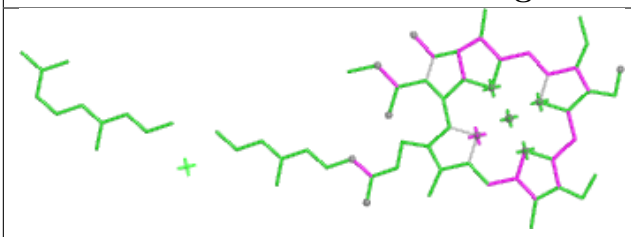


Rings

Ligand CHL BJ 608



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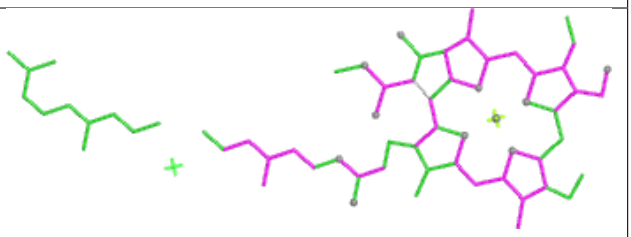

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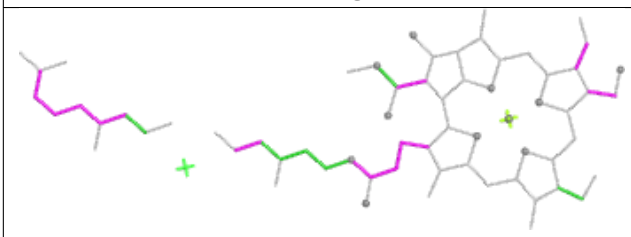

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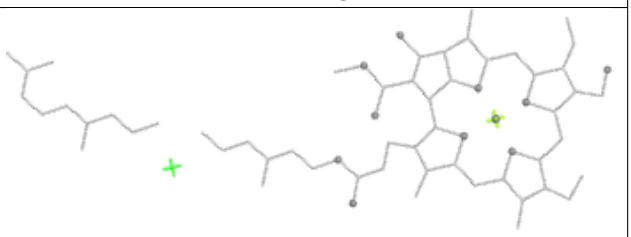
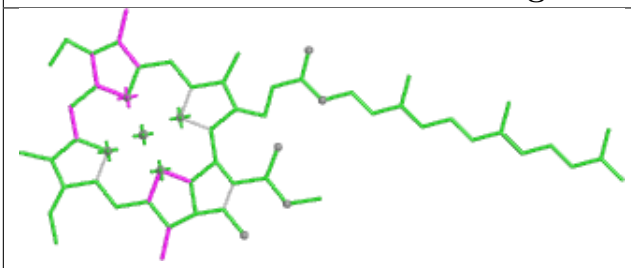
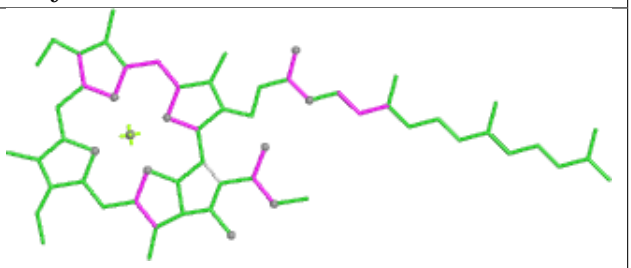


Rings

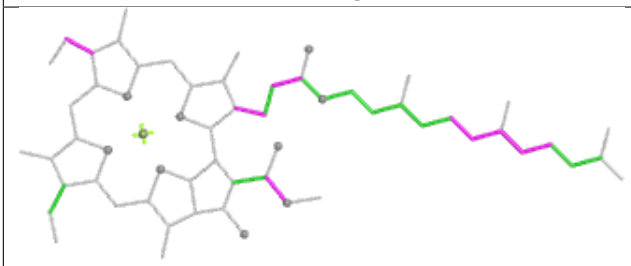
Ligand CLA y 312



Bond lengths



Bond angles



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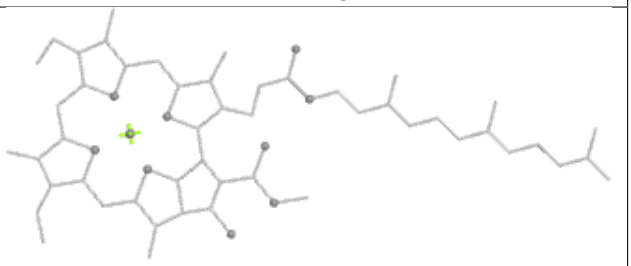
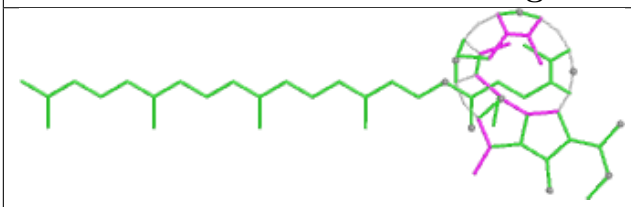


Rings

Ligand PHO a 409



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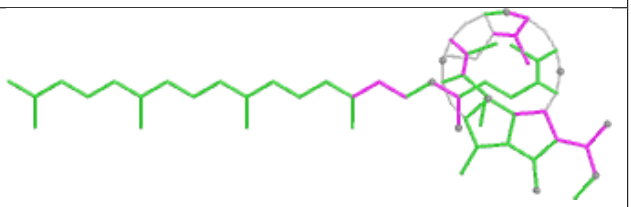
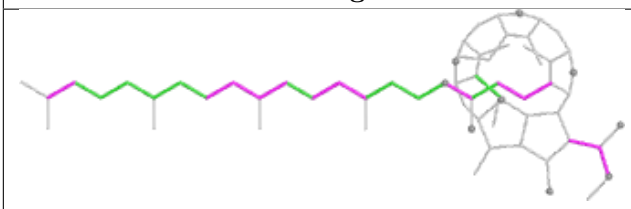


Bond angles



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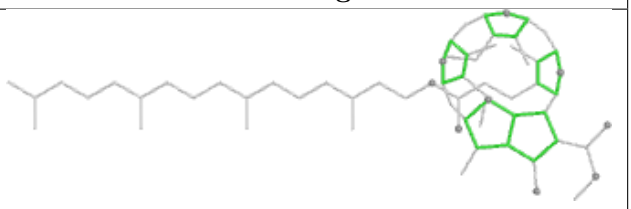
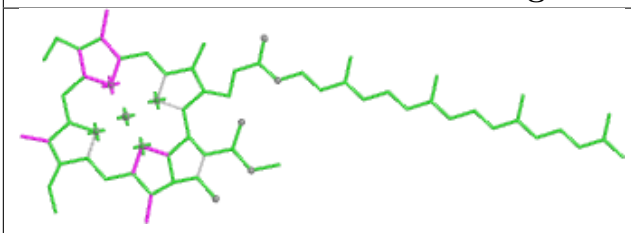
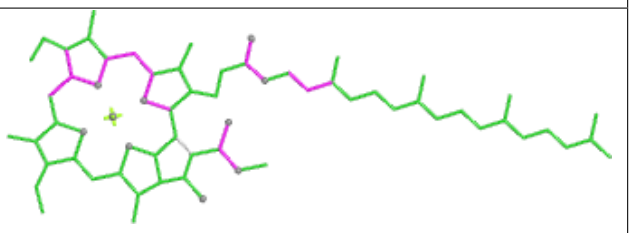


Rings

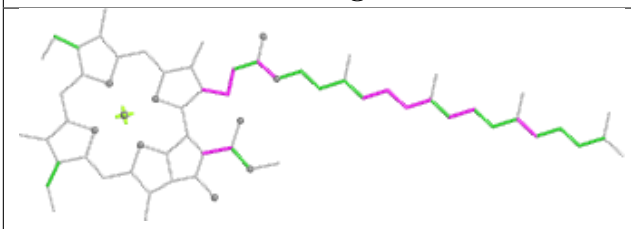
Ligand CLA v 604



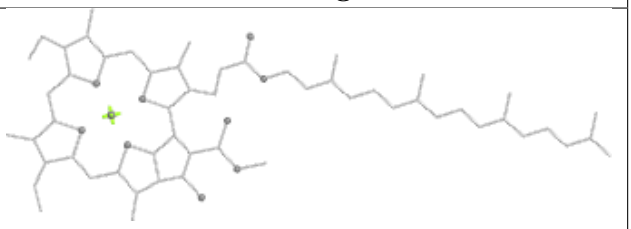
Bond lengths



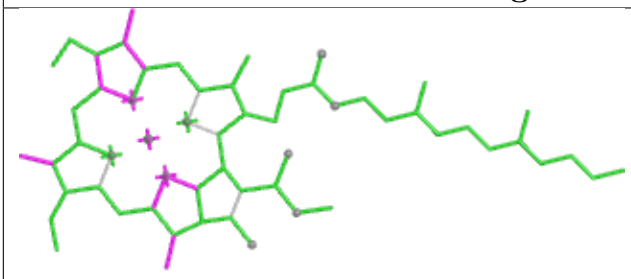
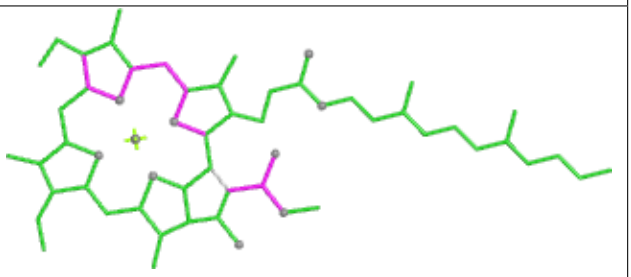
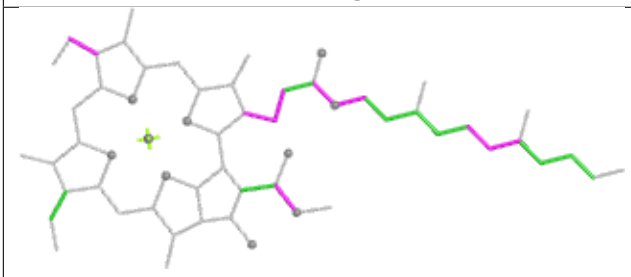
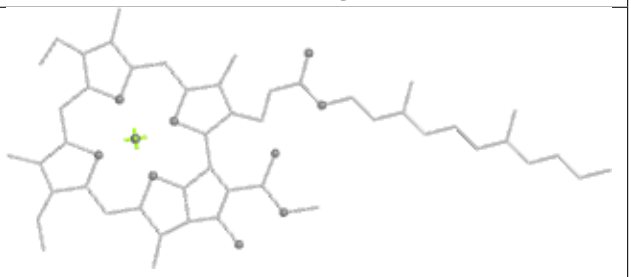
Bond angles

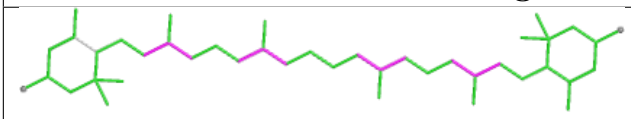
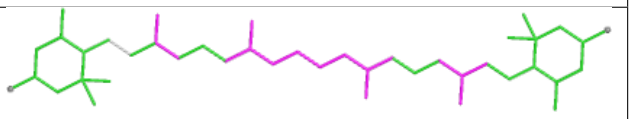
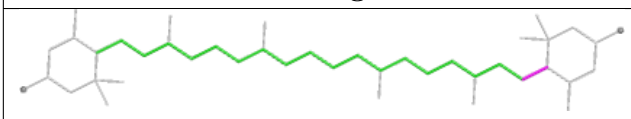
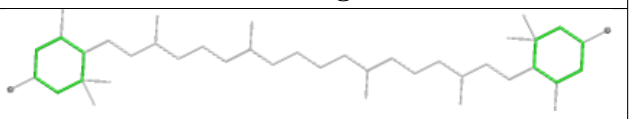


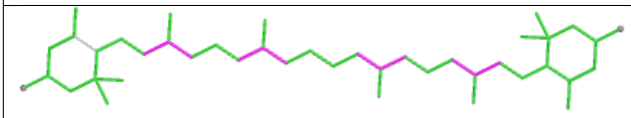
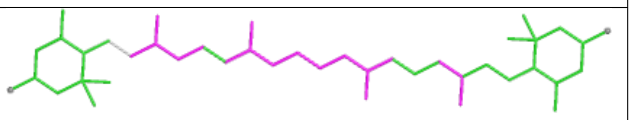
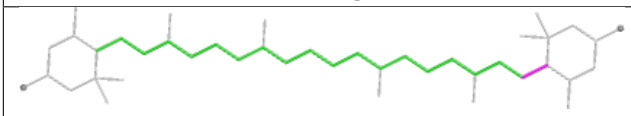
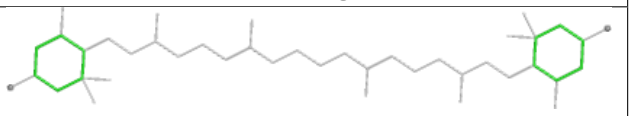
Torsions



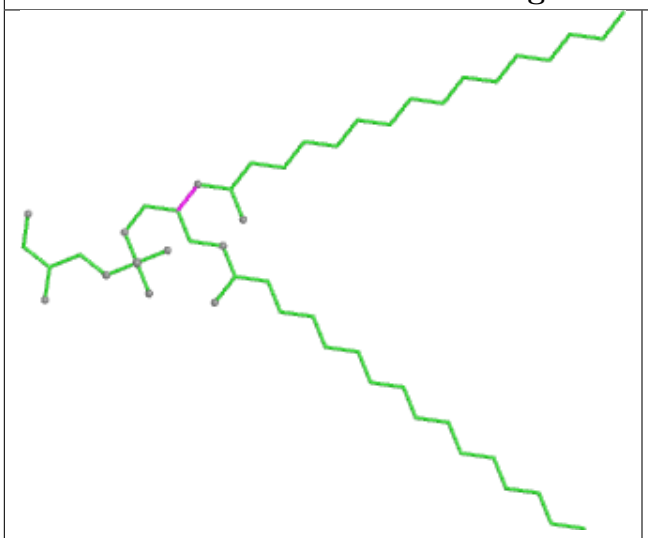
Rings

Ligand CLA BU 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT Au 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT N 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG g 618



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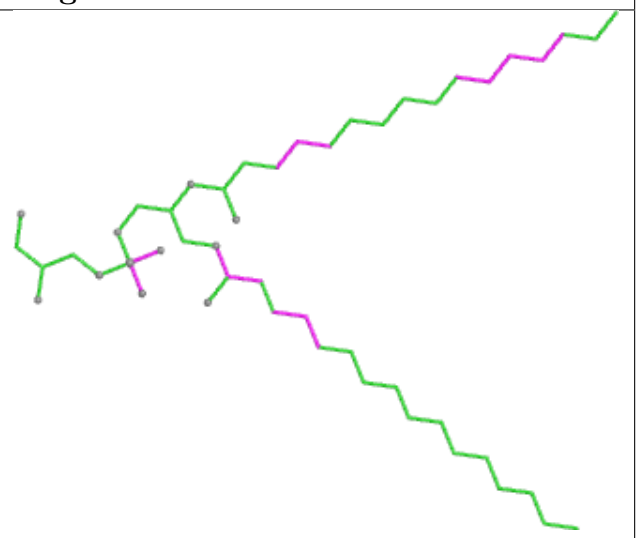

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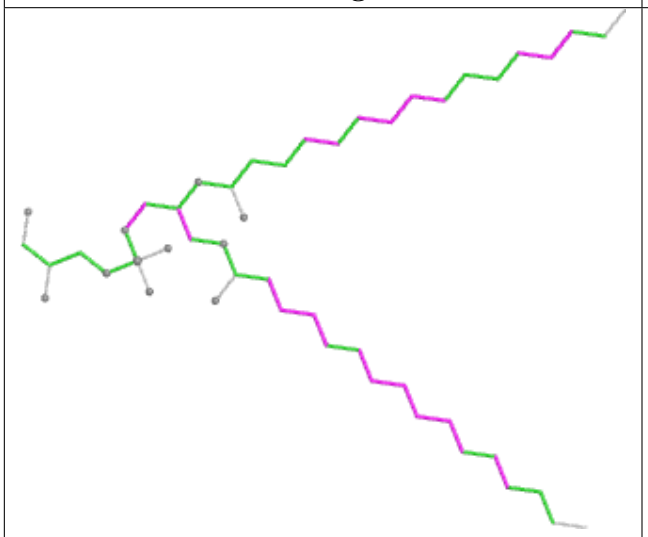

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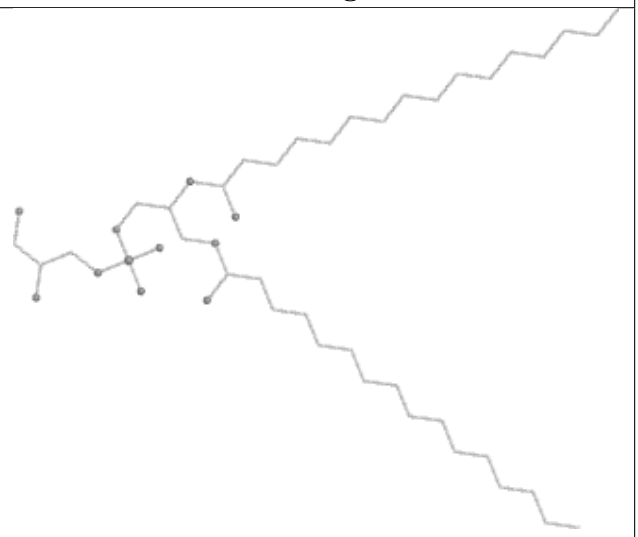
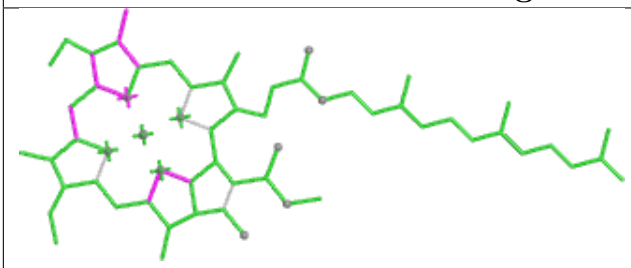


Rings

Ligand CLA BJ 612



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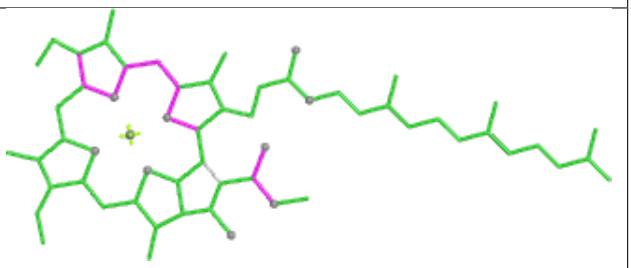

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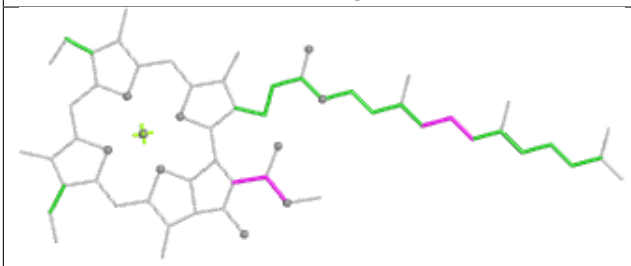

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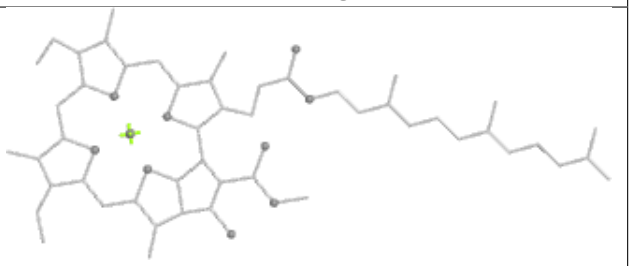
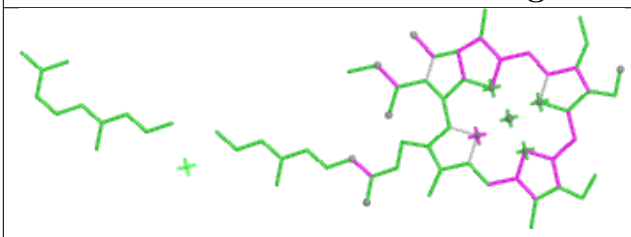


Rings

Ligand CHL y 302



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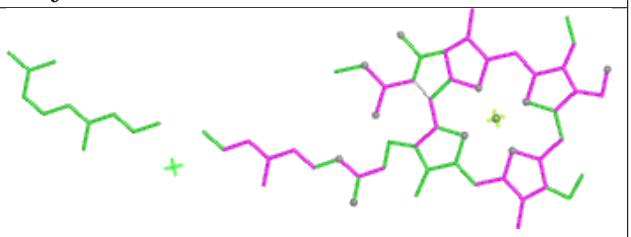

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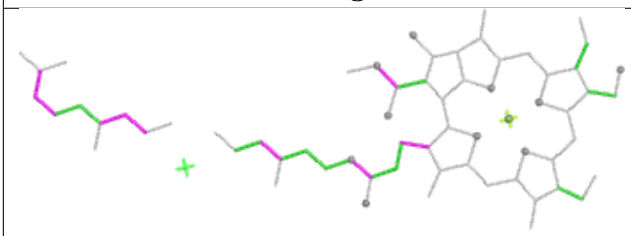

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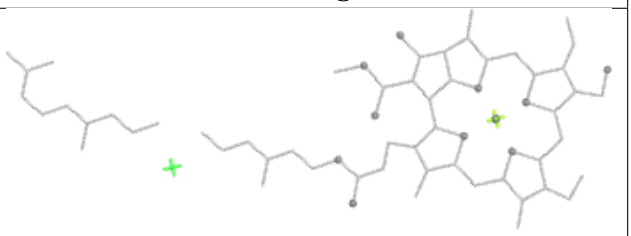
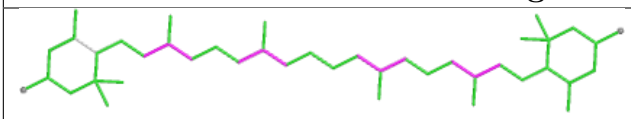


Rings

Ligand LUT S 615



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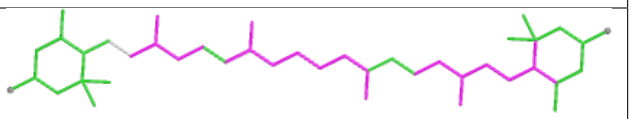
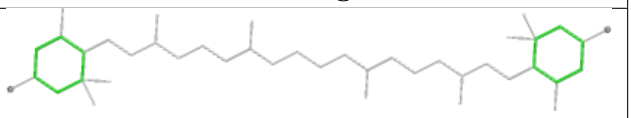


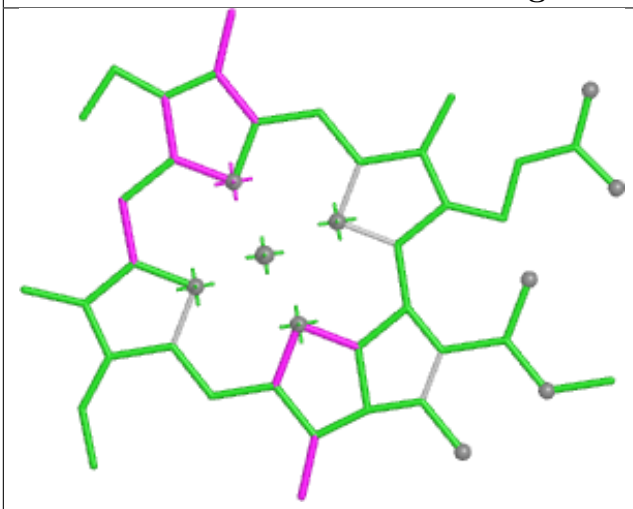
Bond angles

Torsions



Rings

Ligand CLA 5 611



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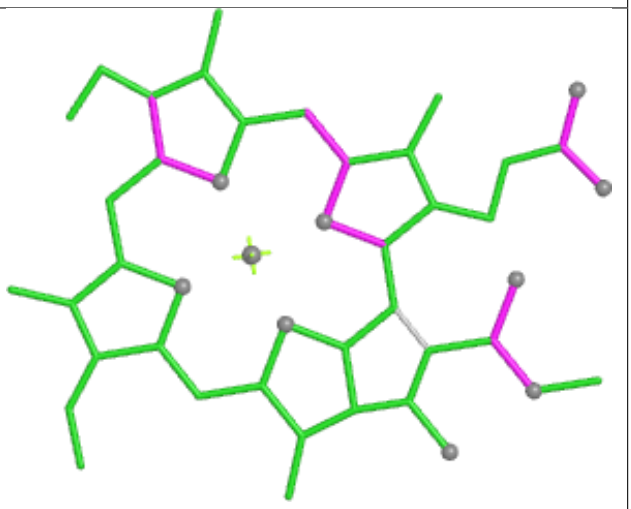

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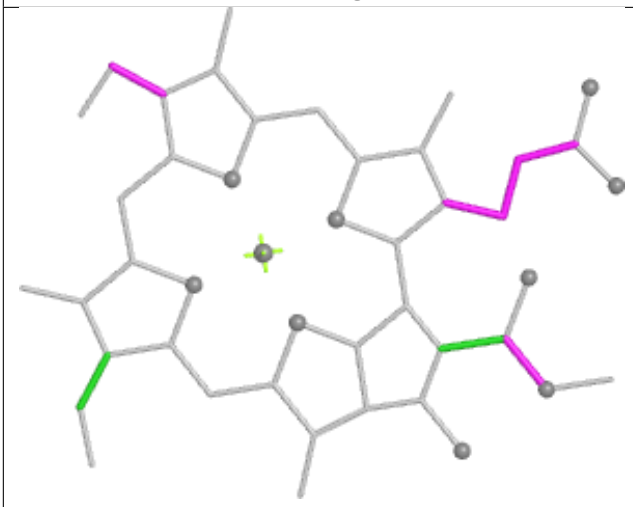
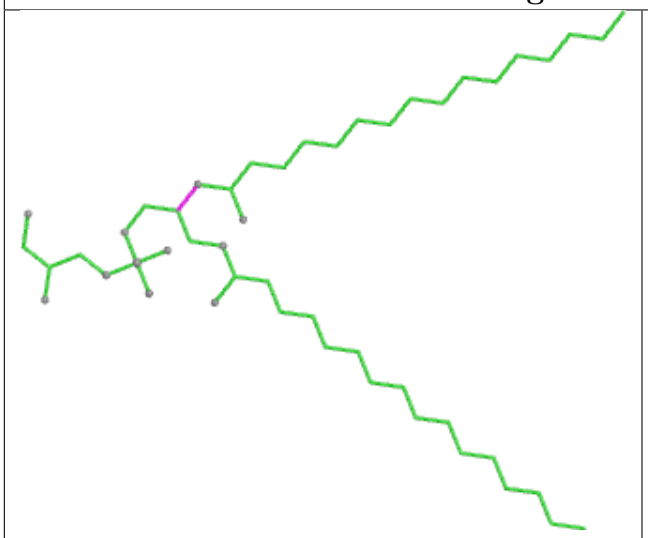


Torsions

Rings

Ligand LHG b 624



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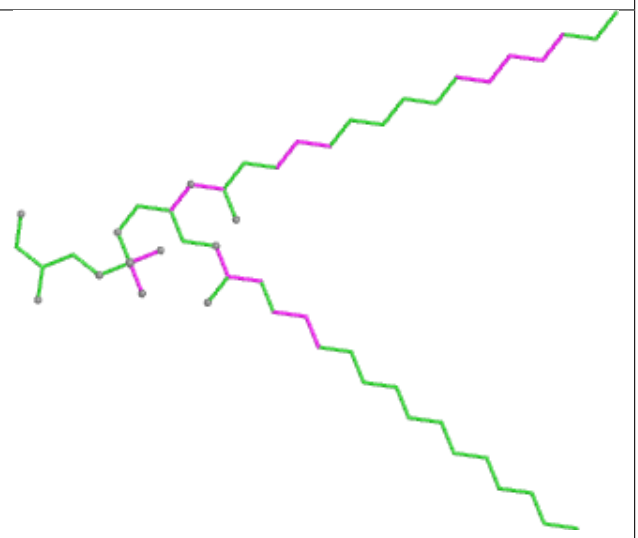
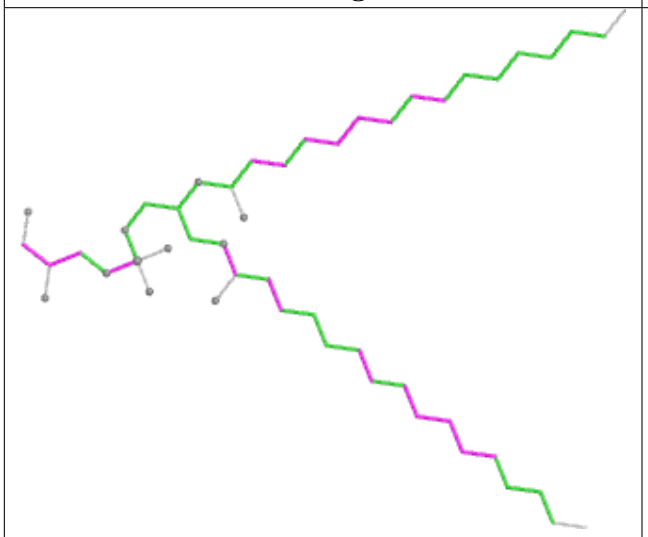


Bond angles



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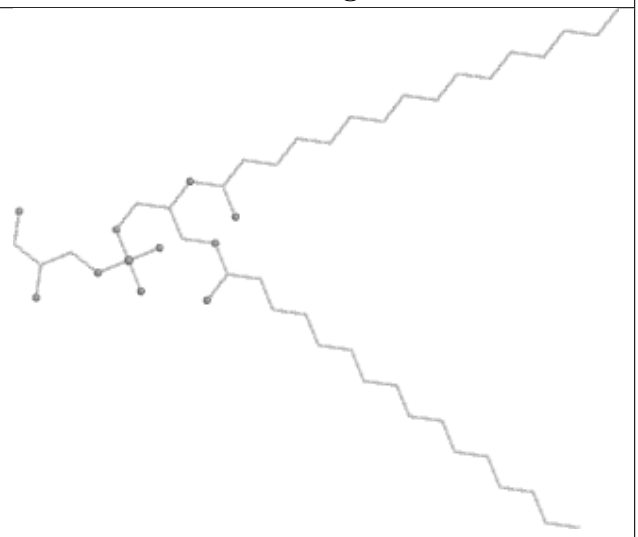
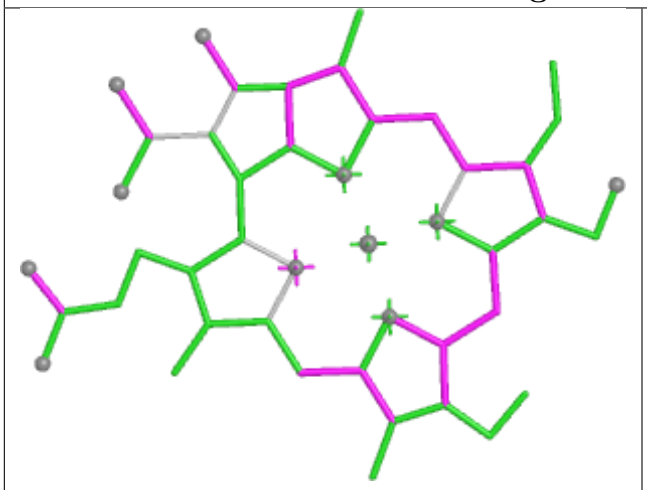


Rings

Ligand CHL e 601



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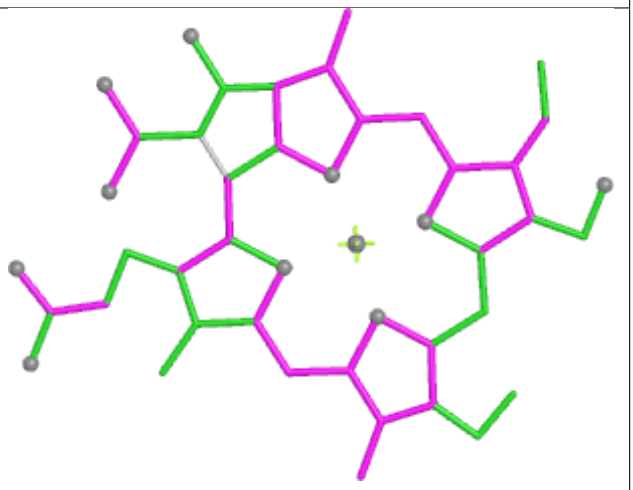

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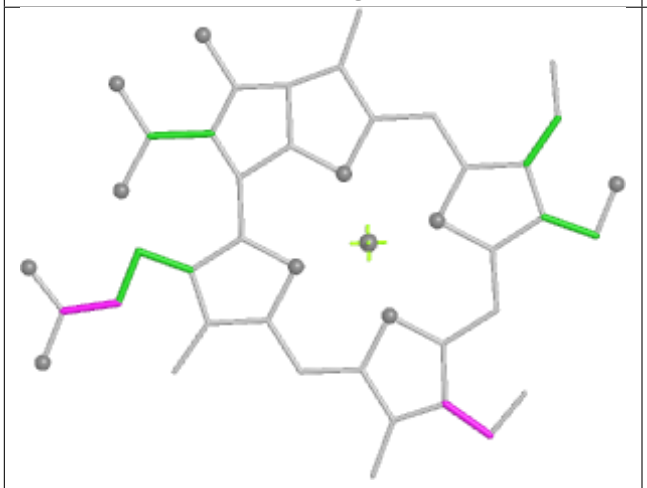
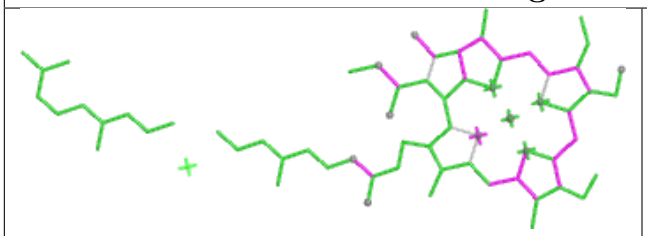


Torsions

Rings

Ligand CHL g 608



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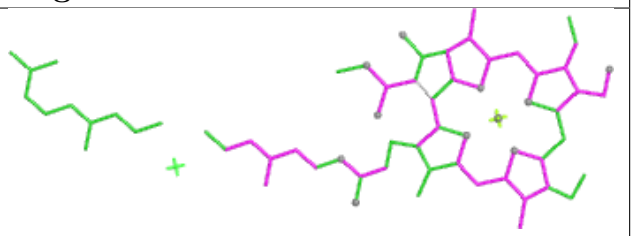

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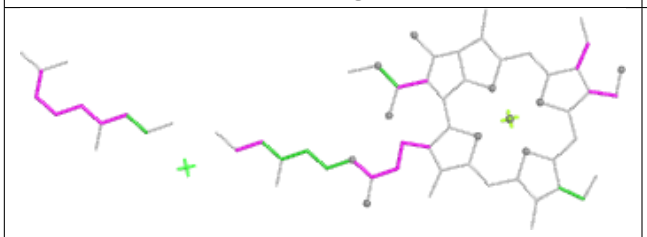

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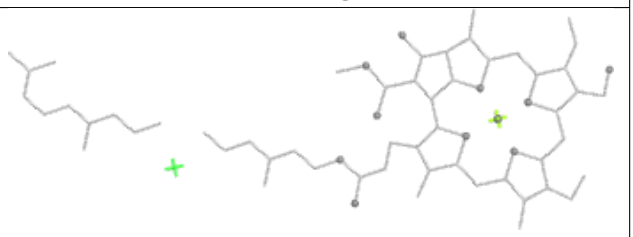
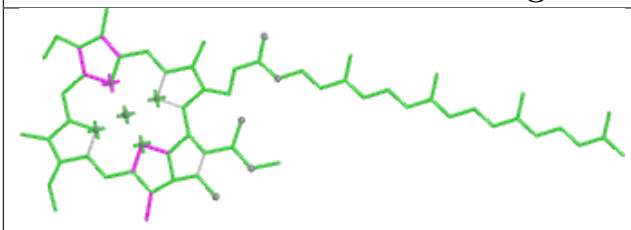
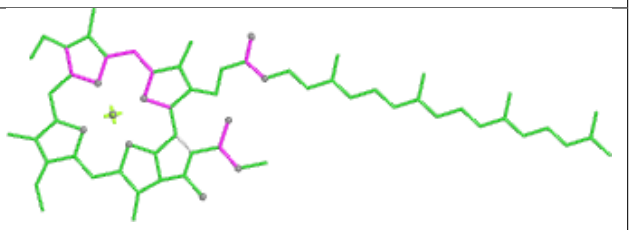
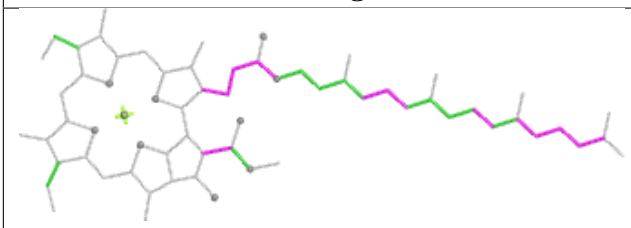
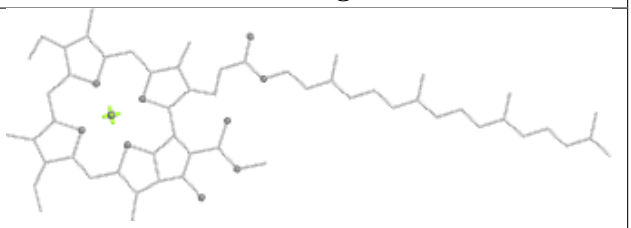
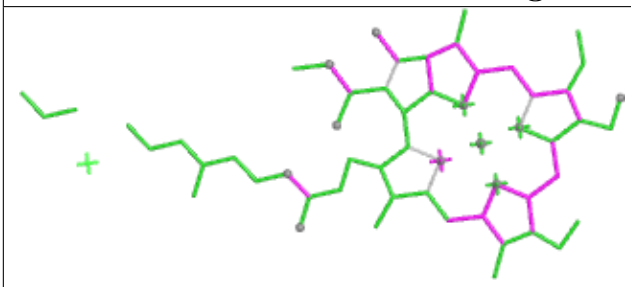
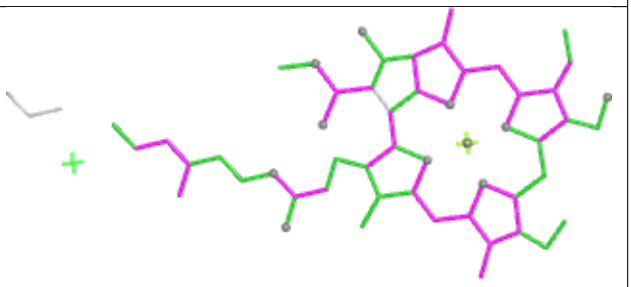
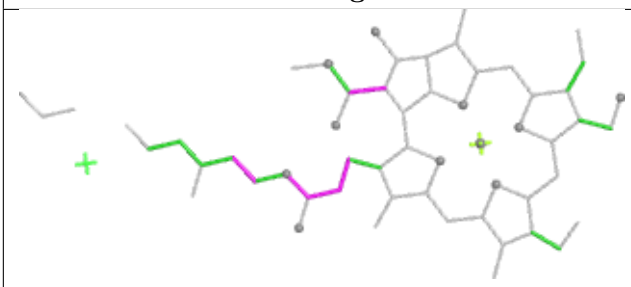
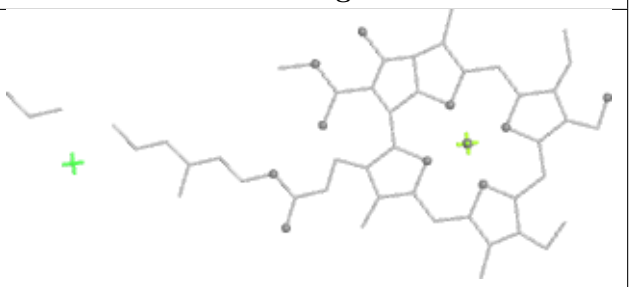
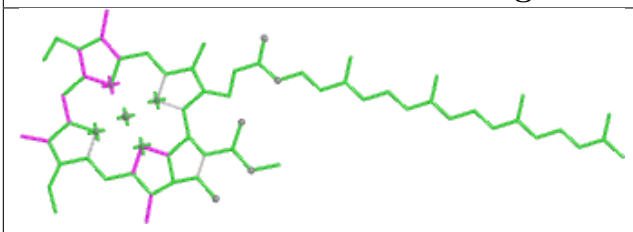


Rings

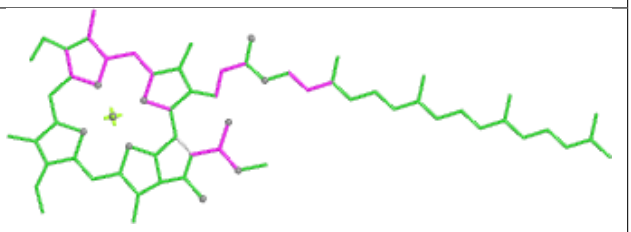
Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL S 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

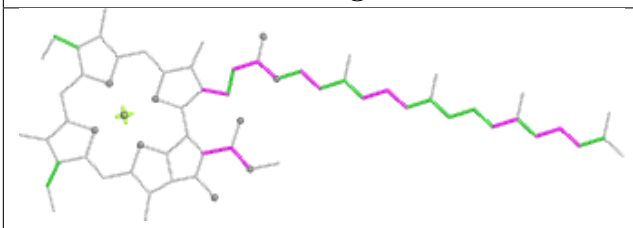
Ligand CLA A2 610



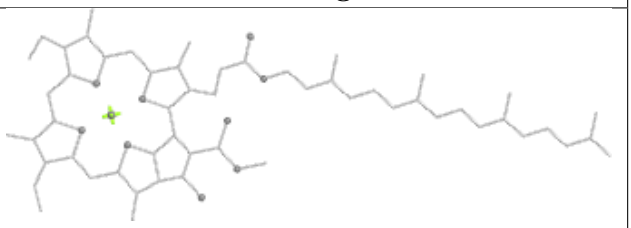
Bond lengths



Bond angles

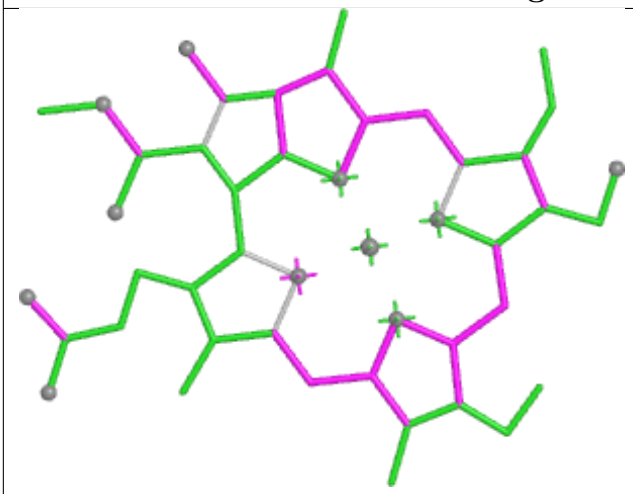


Torsions

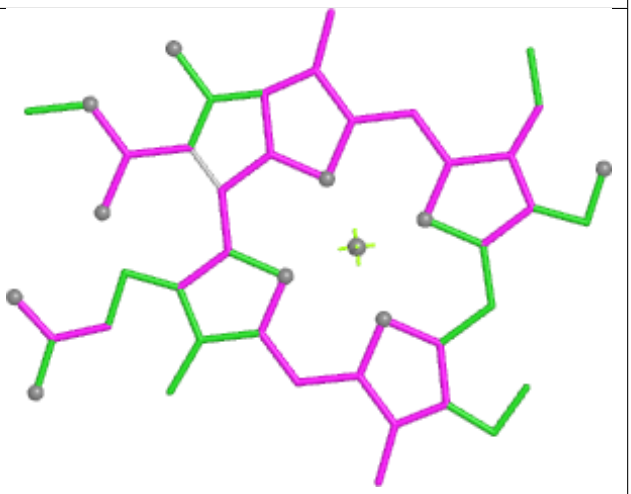


Rings

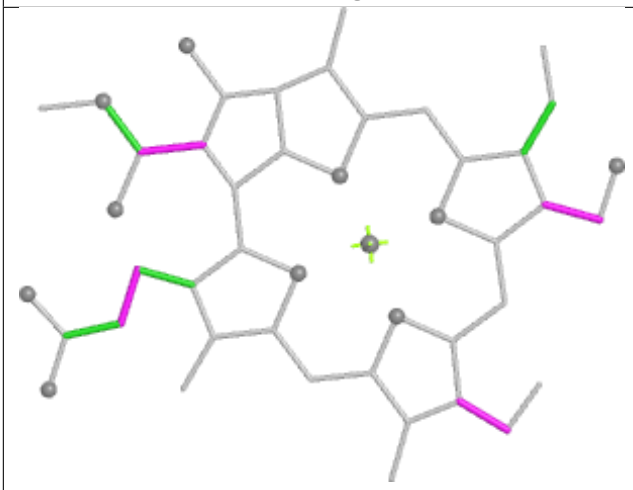
Ligand CHL 9 606



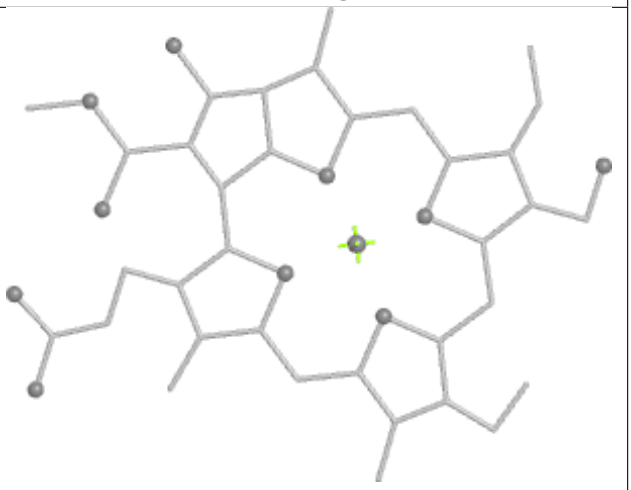
Bond lengths



Bond angles

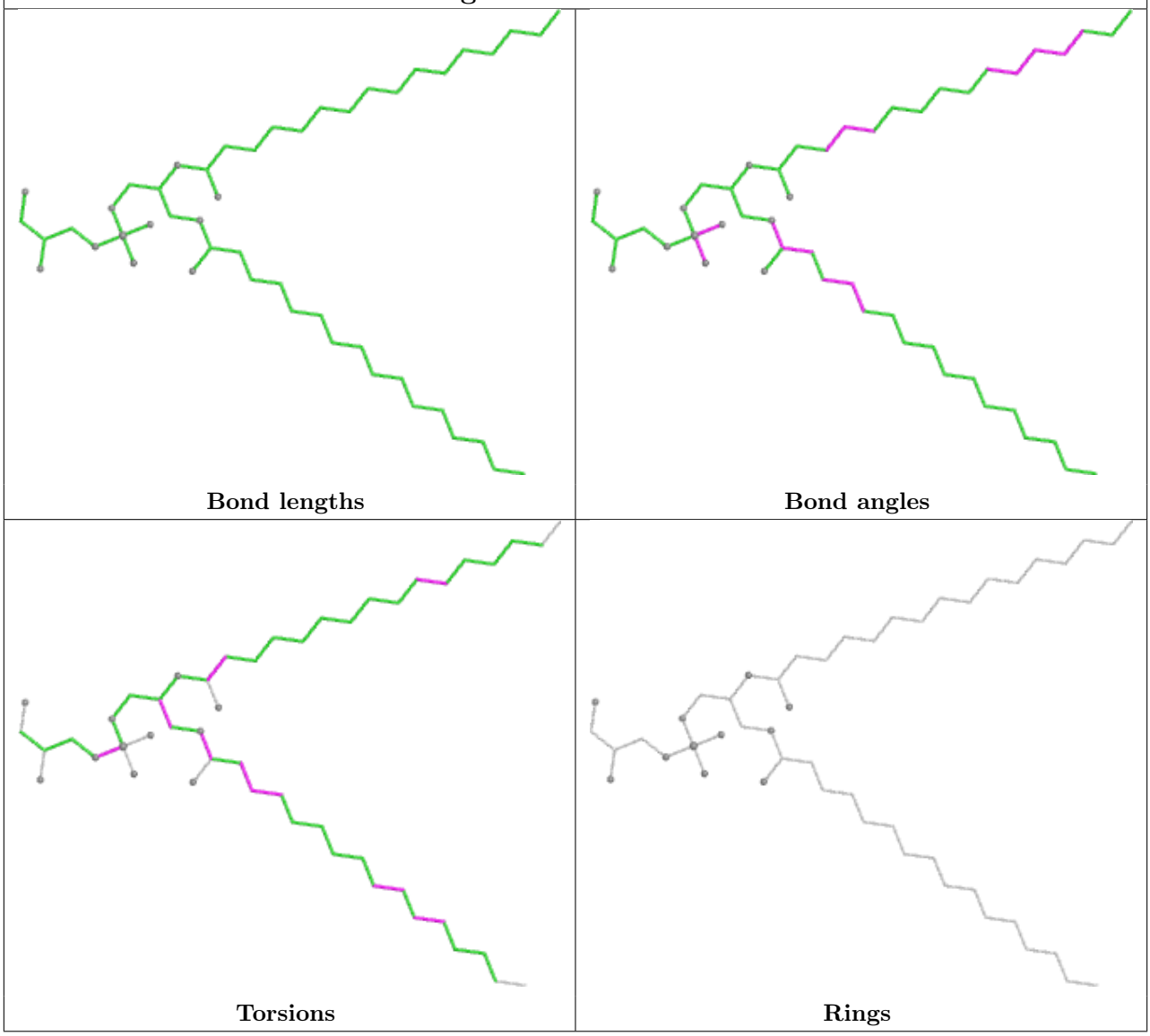


Torsions

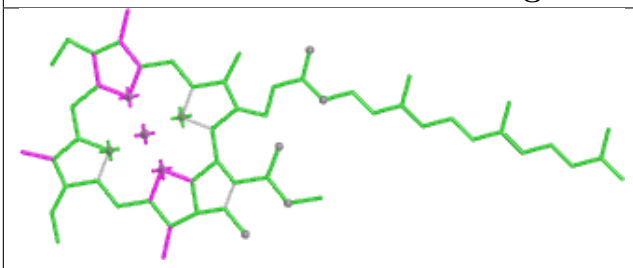


Rings

Ligand LHG A0 202



Ligand CLA Y 311



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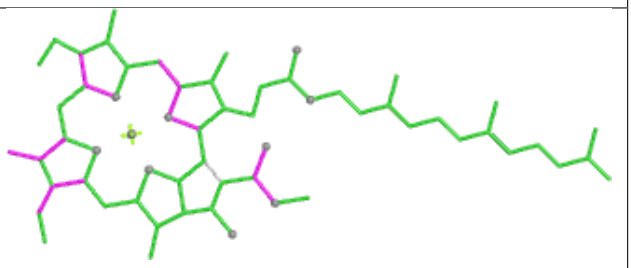

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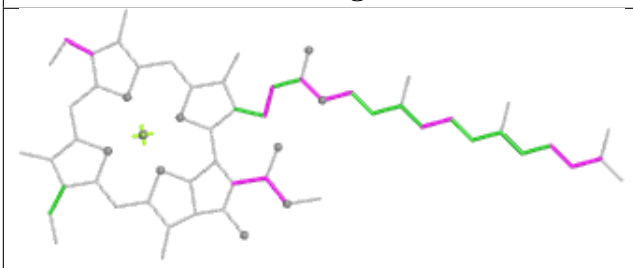

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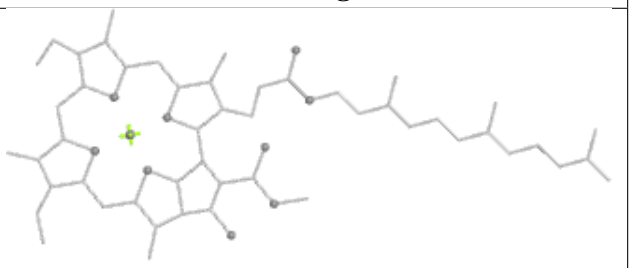
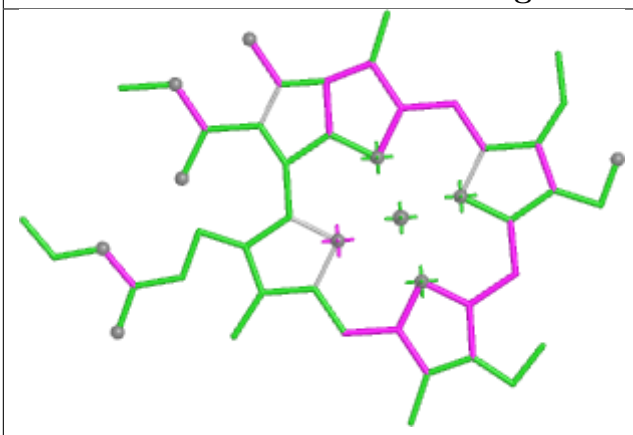


Rings

Ligand CHL A2 605



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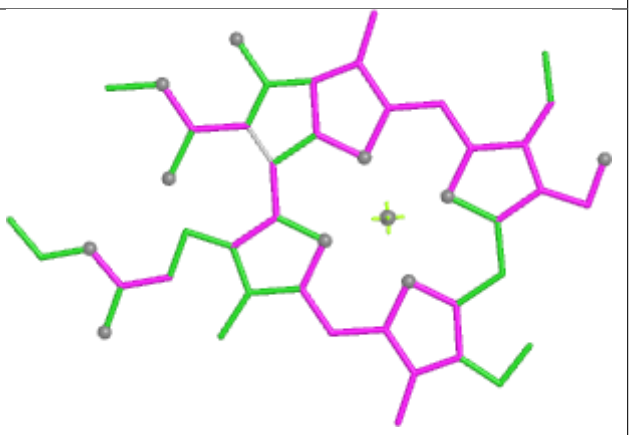

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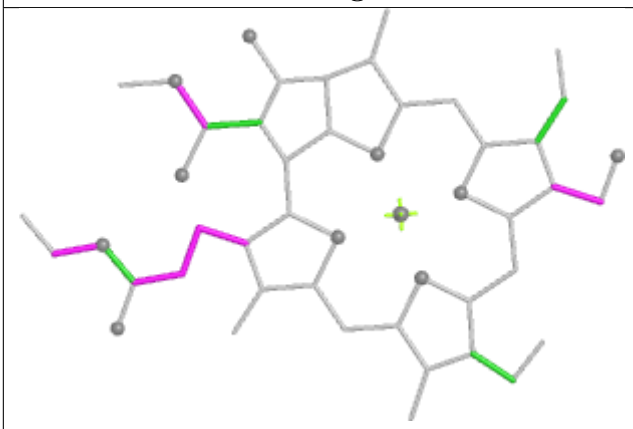

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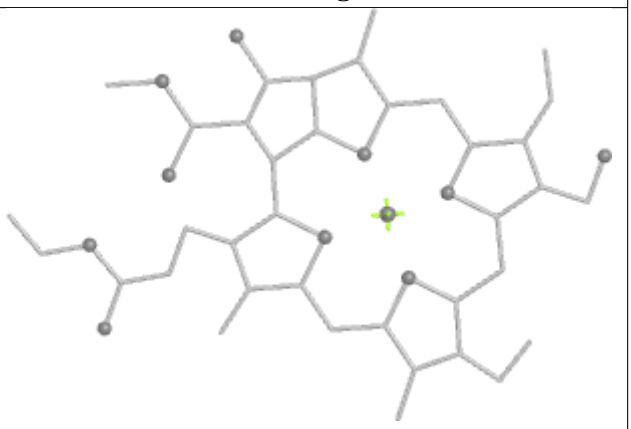
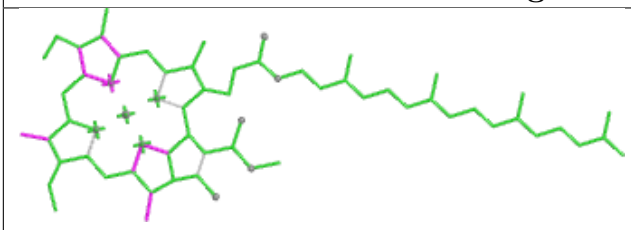


Rings

Ligand CLA b 617



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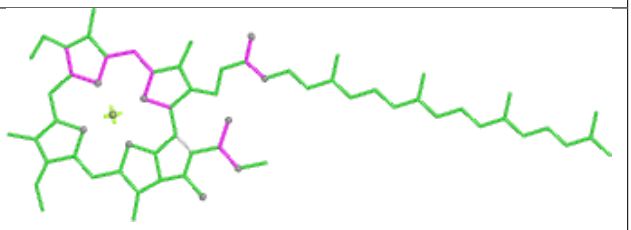

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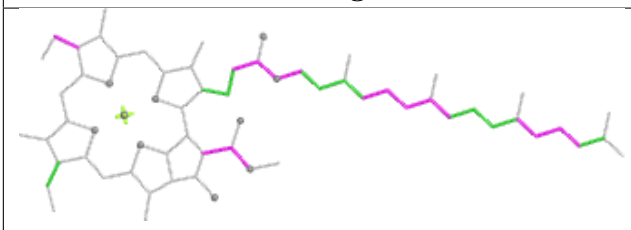

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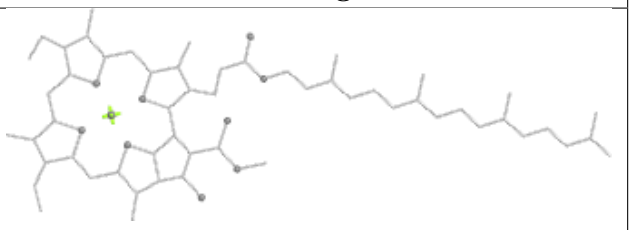
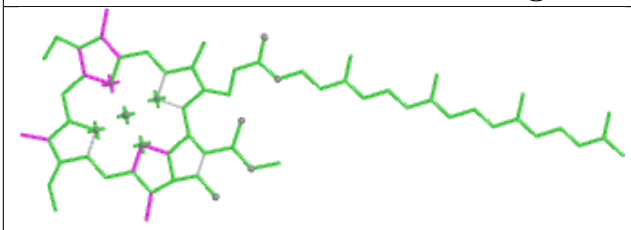


Rings

Ligand CLA v 616



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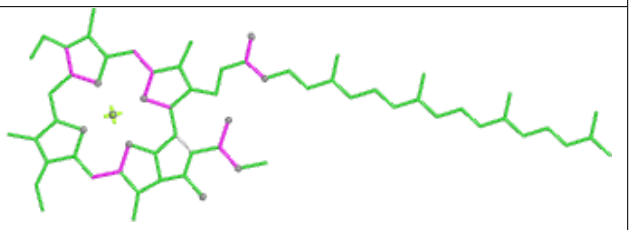

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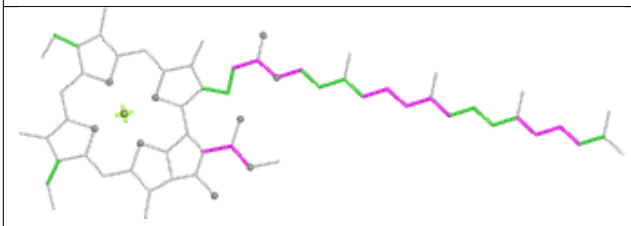

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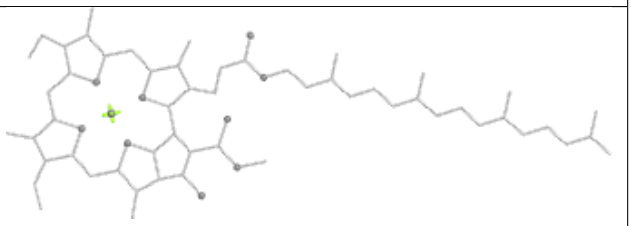
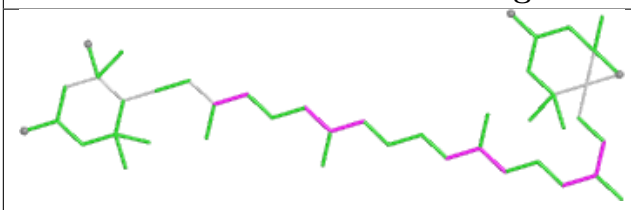


Rings

Ligand NEX Ba 318



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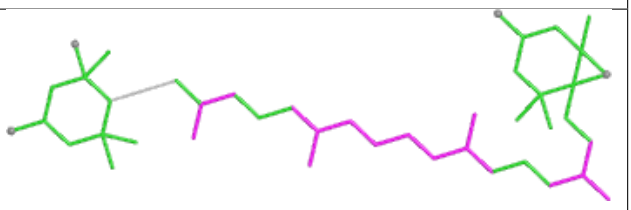

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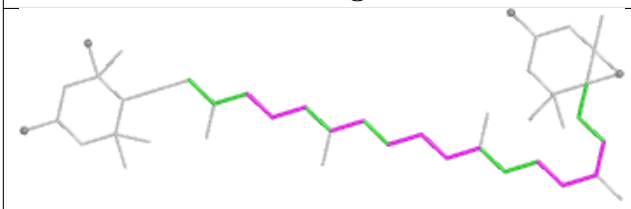
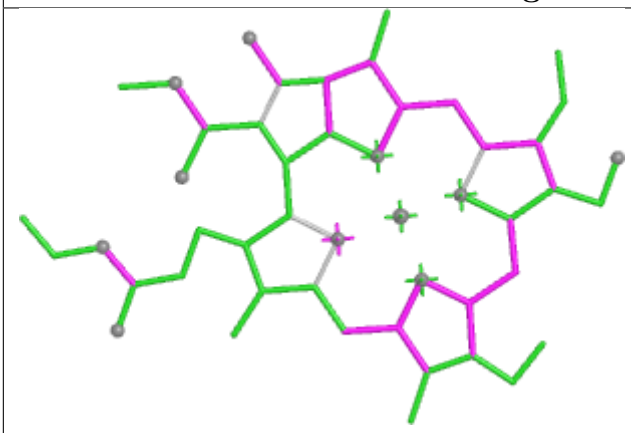
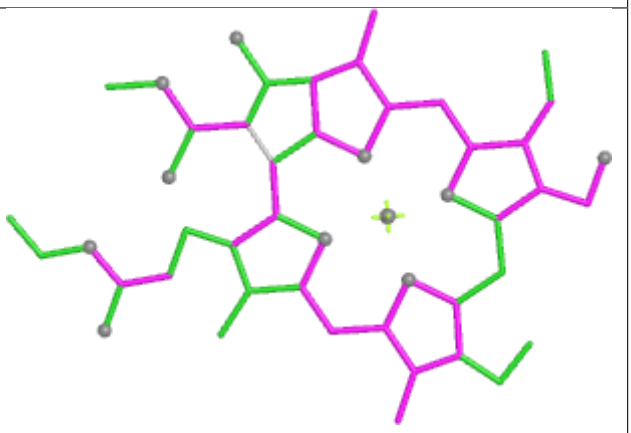
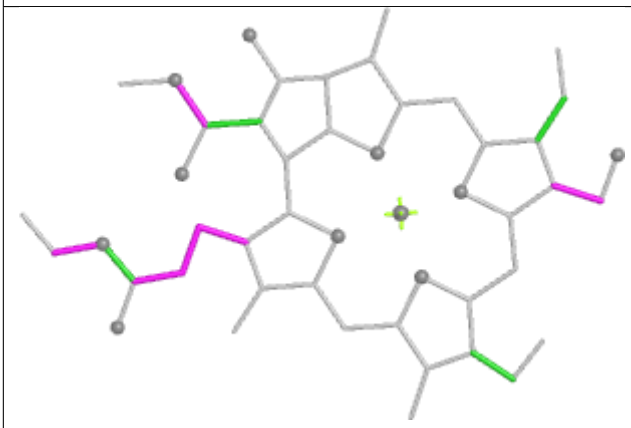
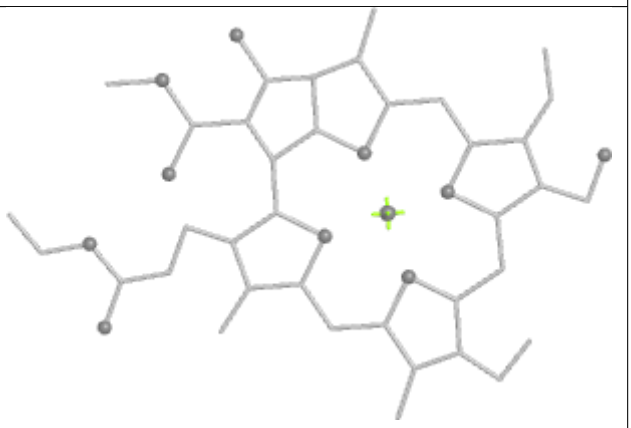


Torsions

Rings

Ligand CHL N 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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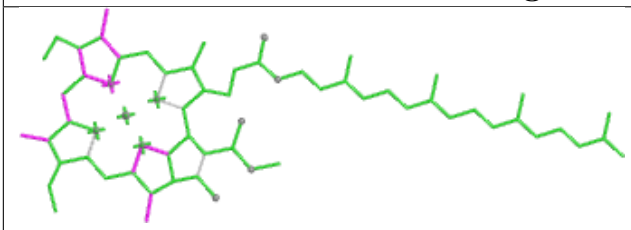
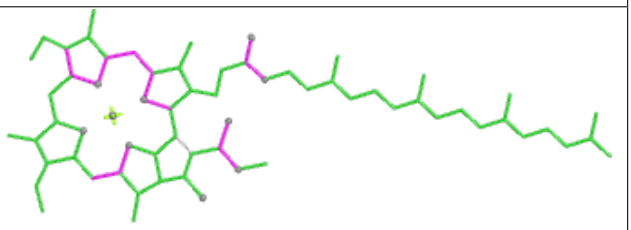
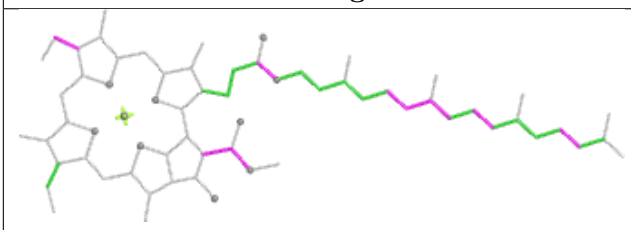
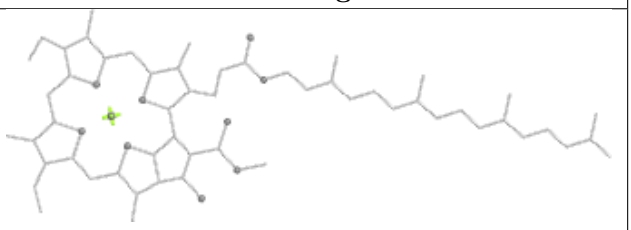
 Bond lengths	 Bond angles
 Torsions	 Rings

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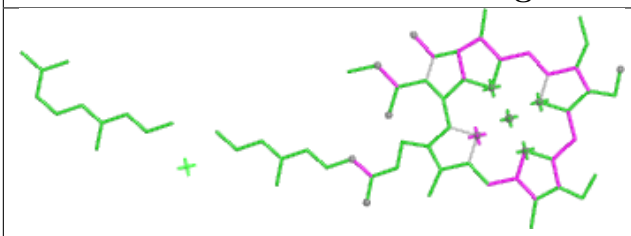
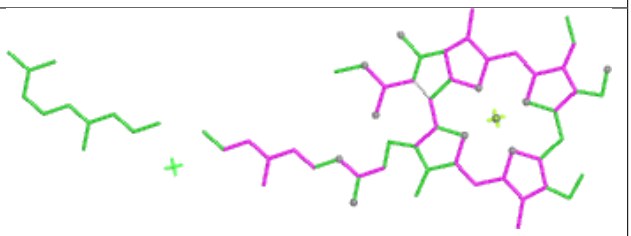
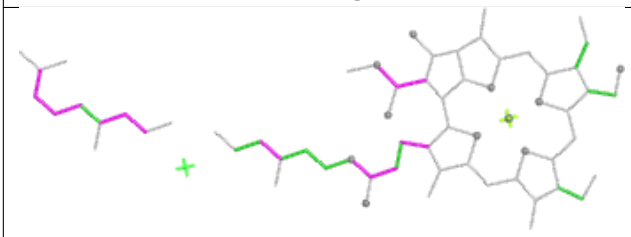
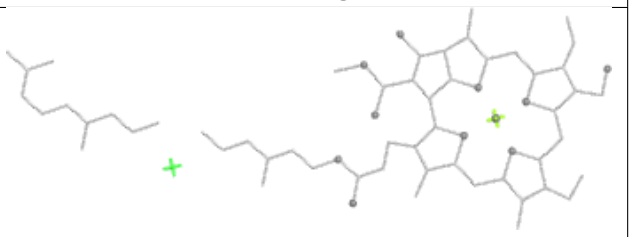
 Bond lengths	 Bond angles
 Torsions	 Rings

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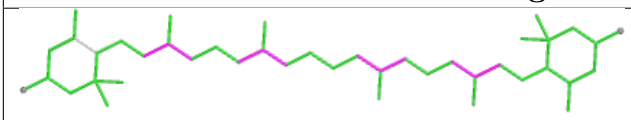
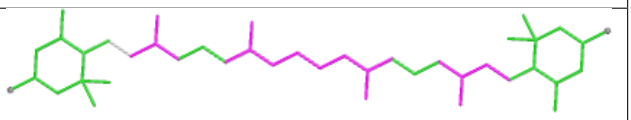
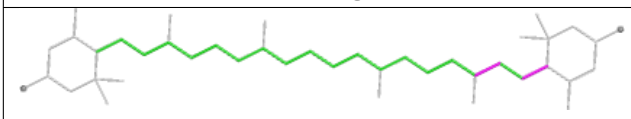
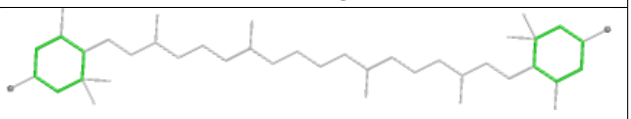
 Bond lengths	 Bond angles
 Torsions	 Rings

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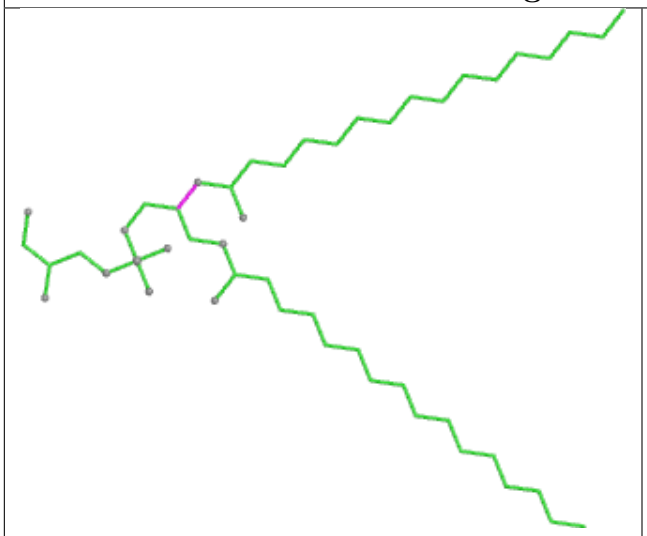
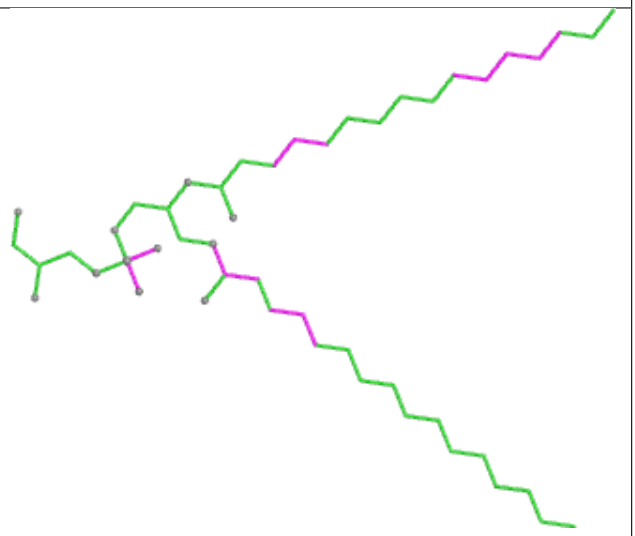
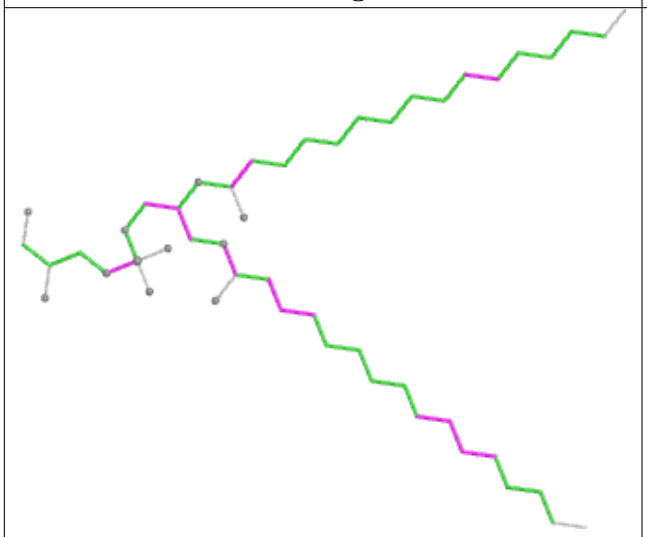
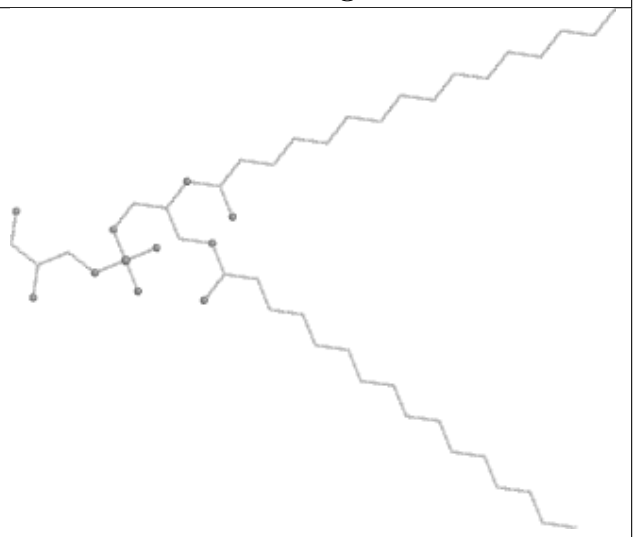
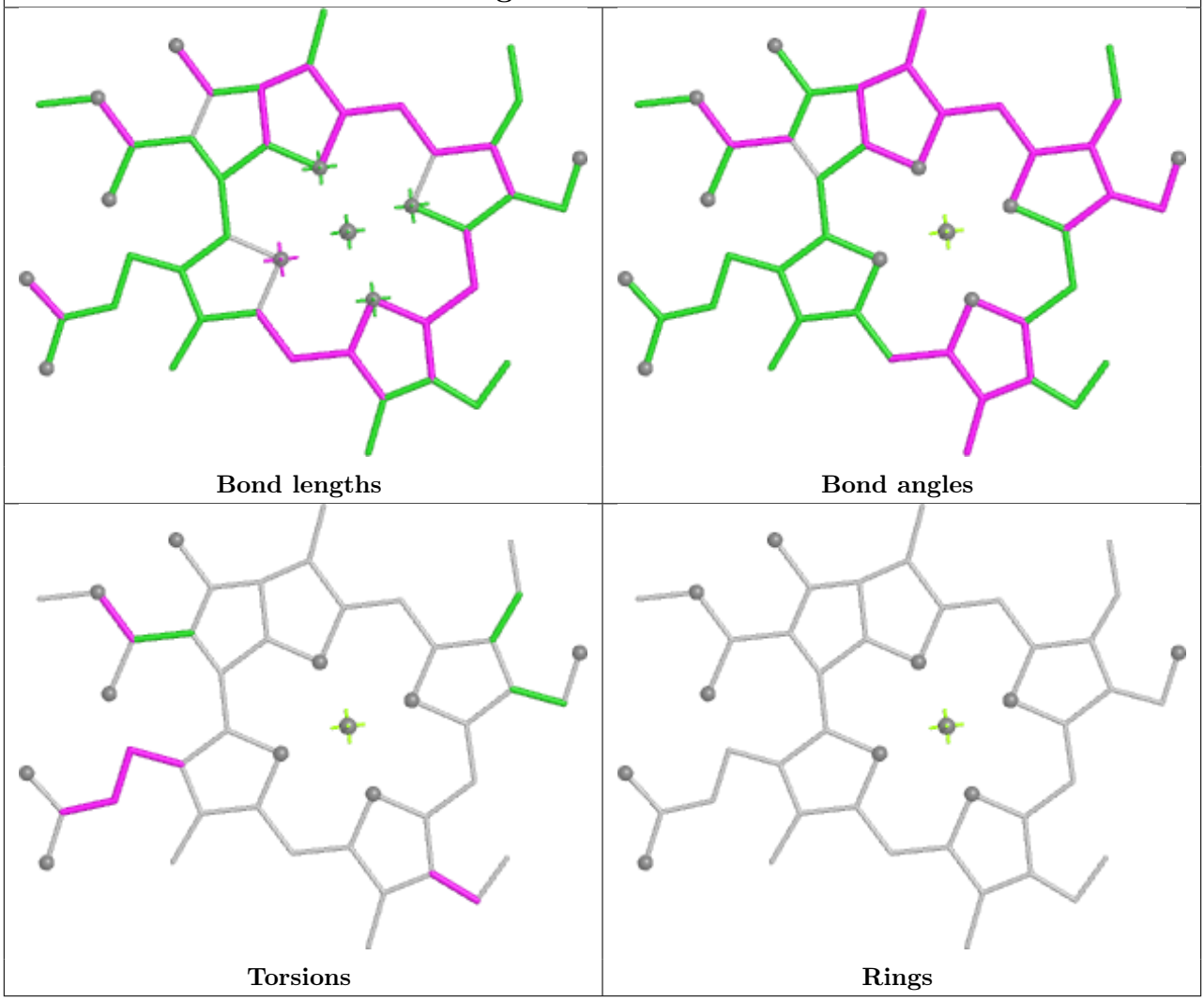
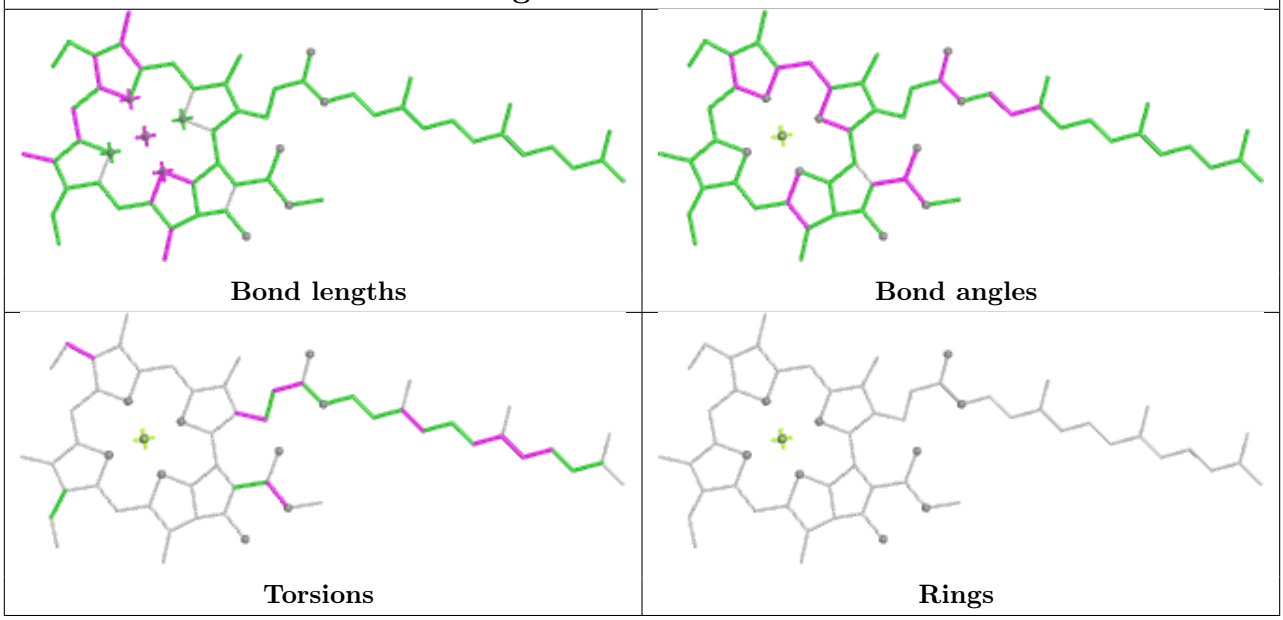
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 8 305



Ligand CLA BB 312



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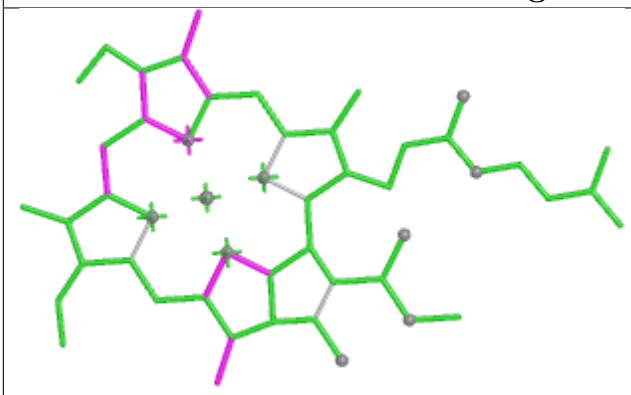
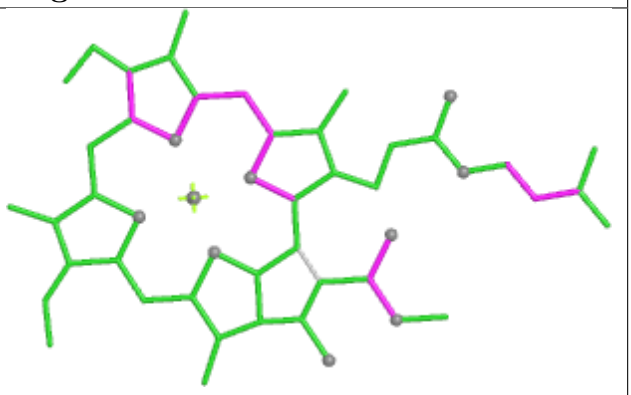
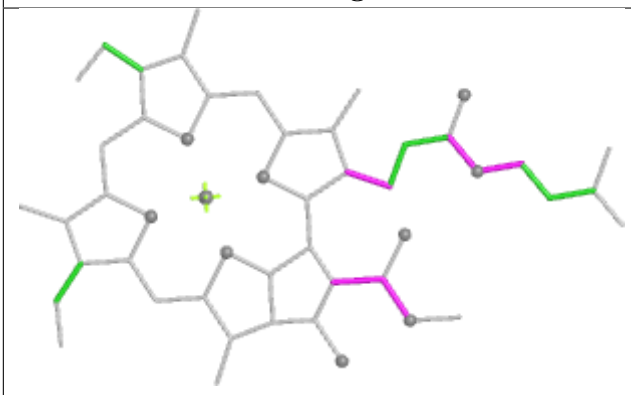
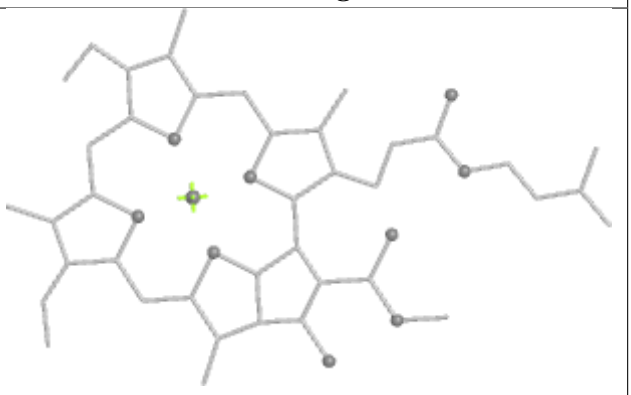
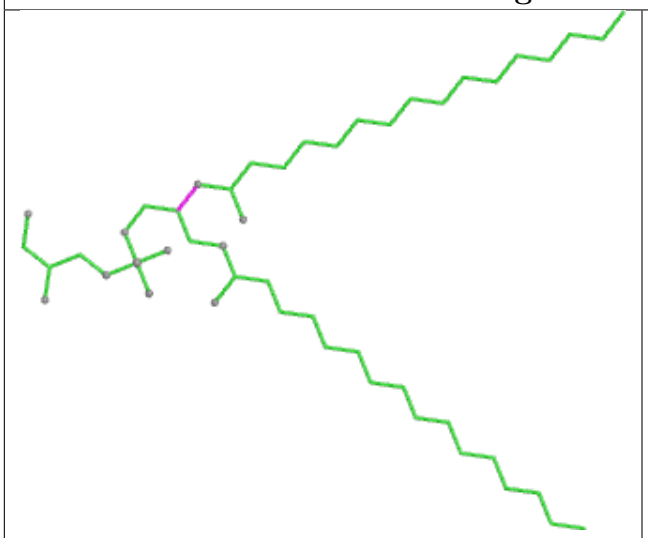
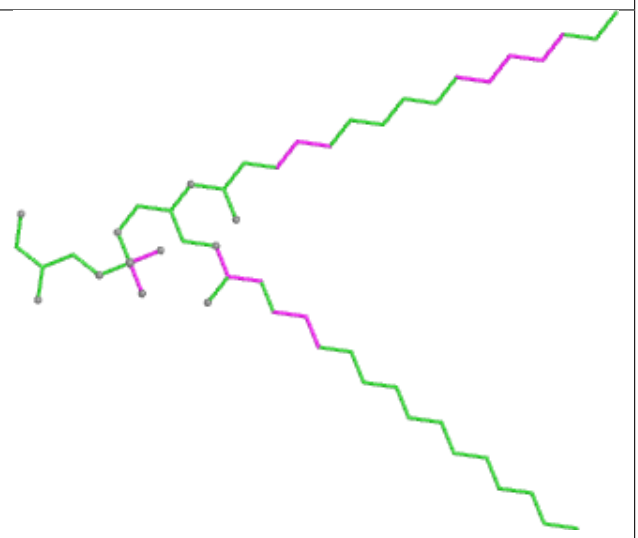
 Bond lengths	 Bond angles
 Torsions	 Rings

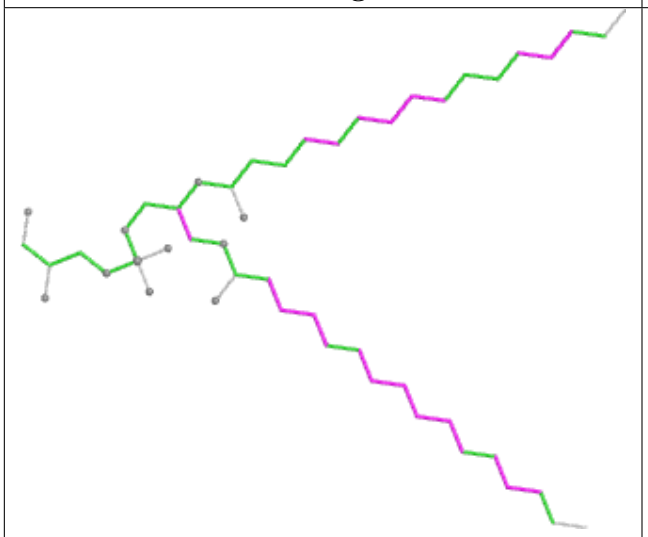
Ligand LHG BJ 618



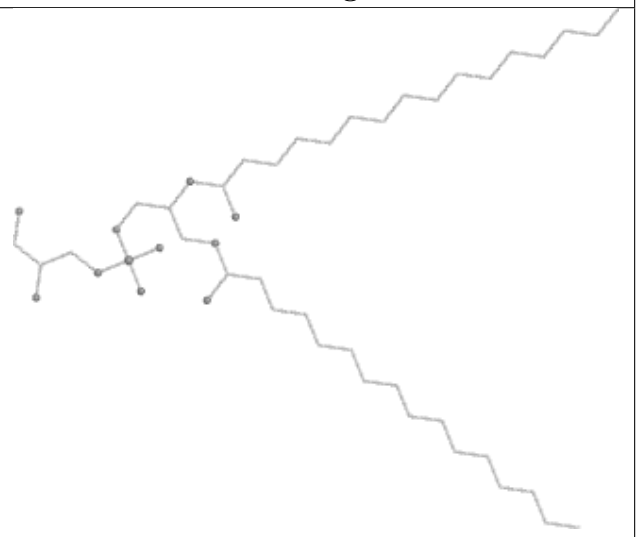
Bond lengths



Bond angles

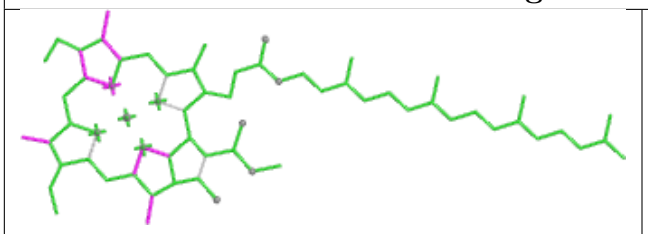


Torsions



Rings

Ligand CLA B 616



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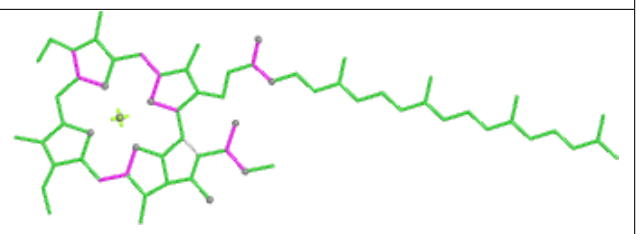
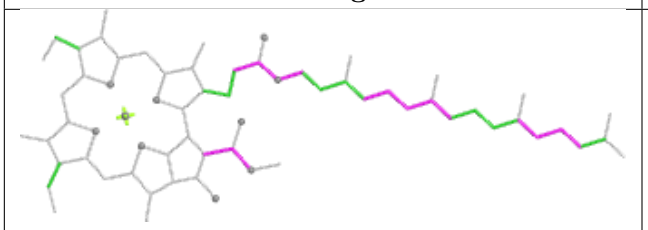
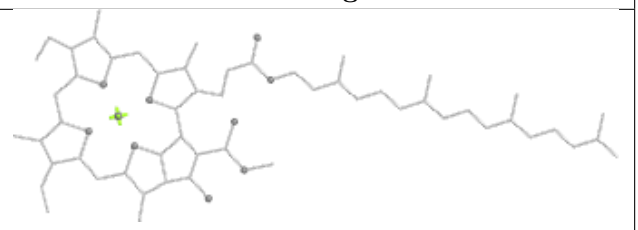


Bond angles

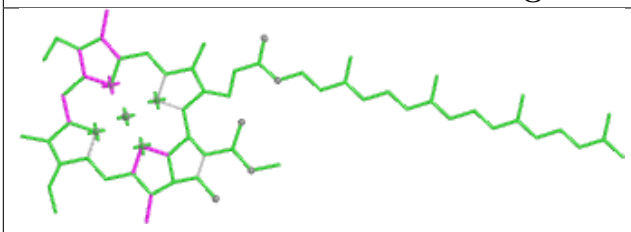


Torsions

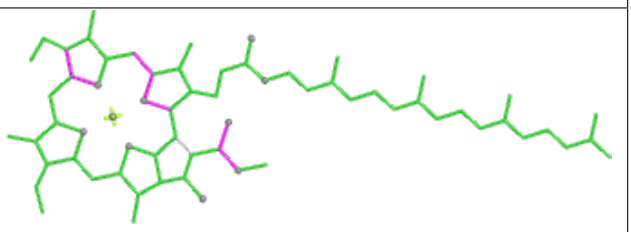


Rings

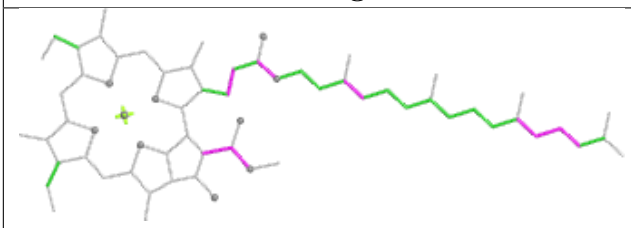
Ligand CLA B 603



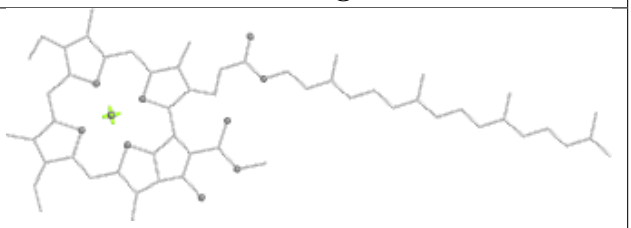
Bond lengths



Bond angles

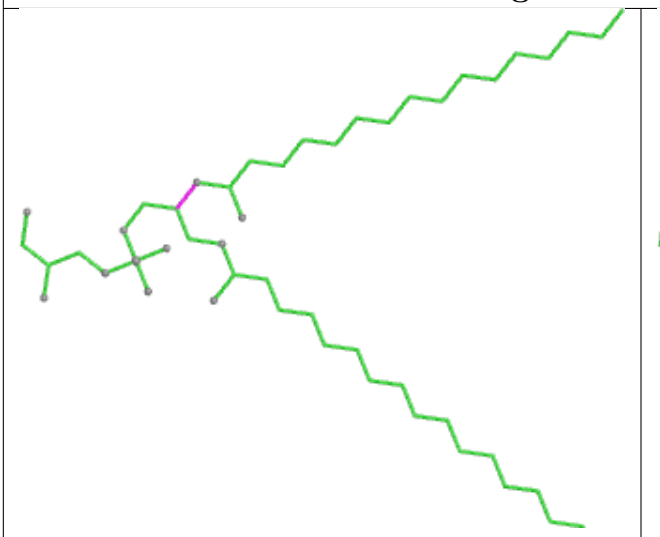


Torsions



Rings

Ligand LHG BF 521



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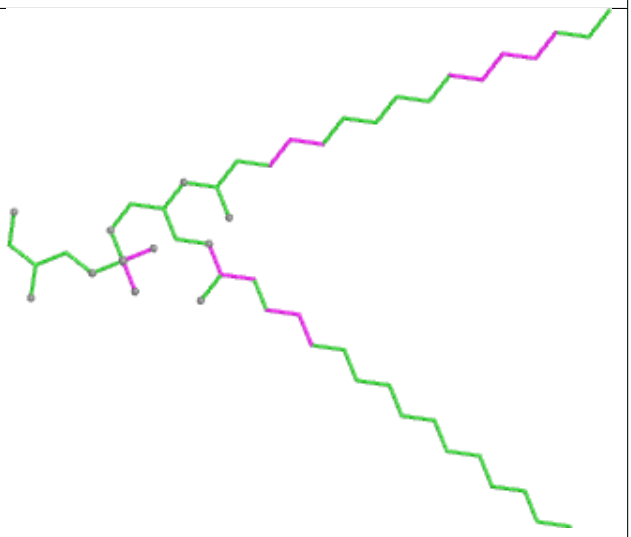

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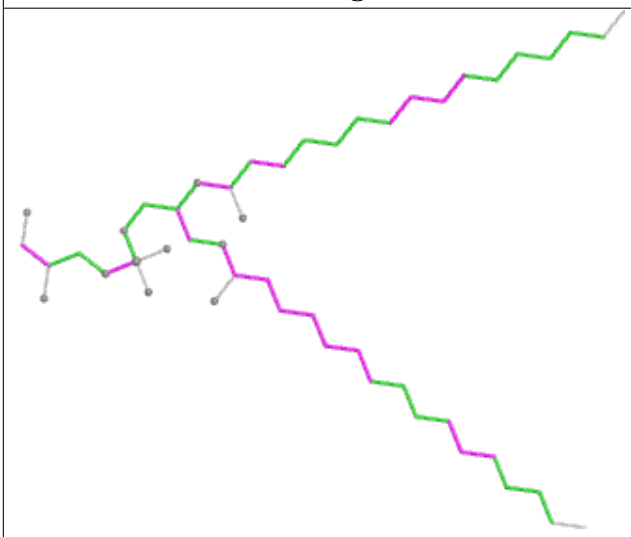

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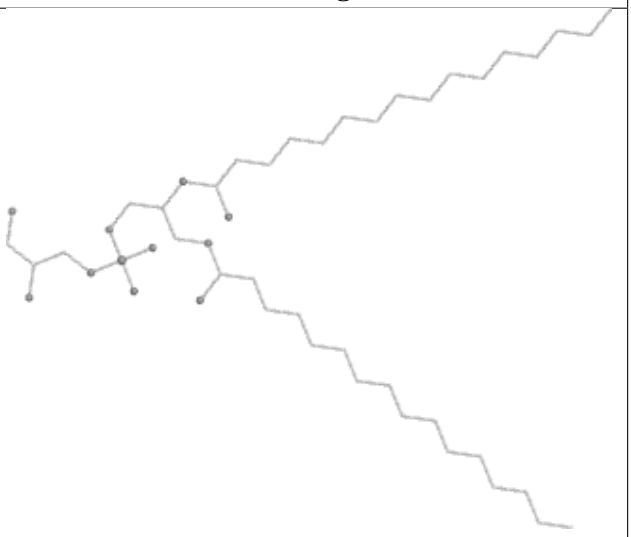
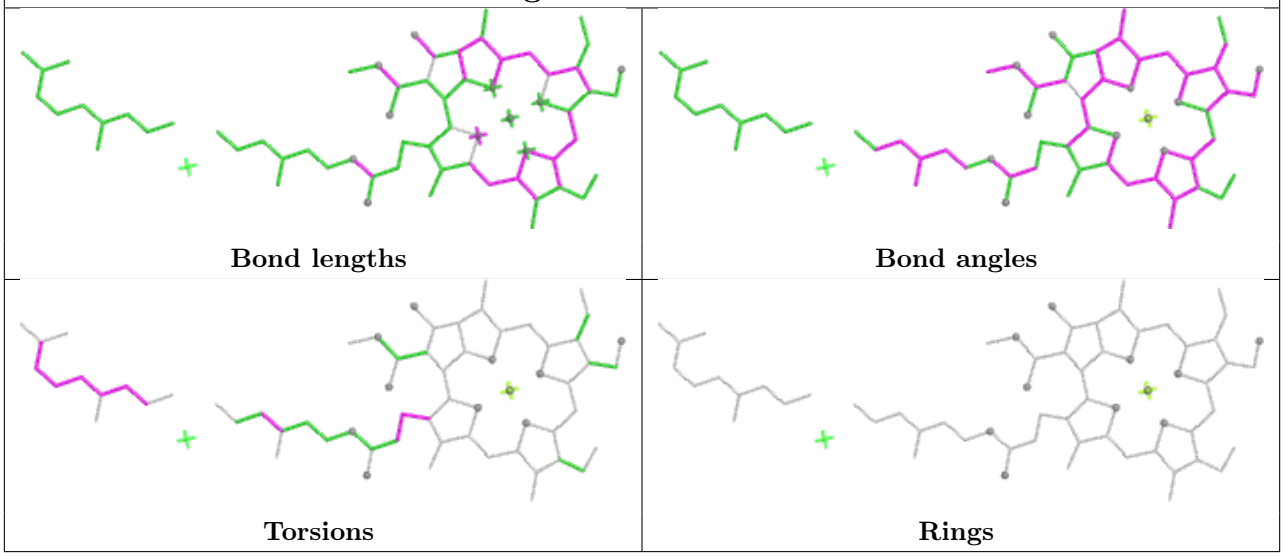
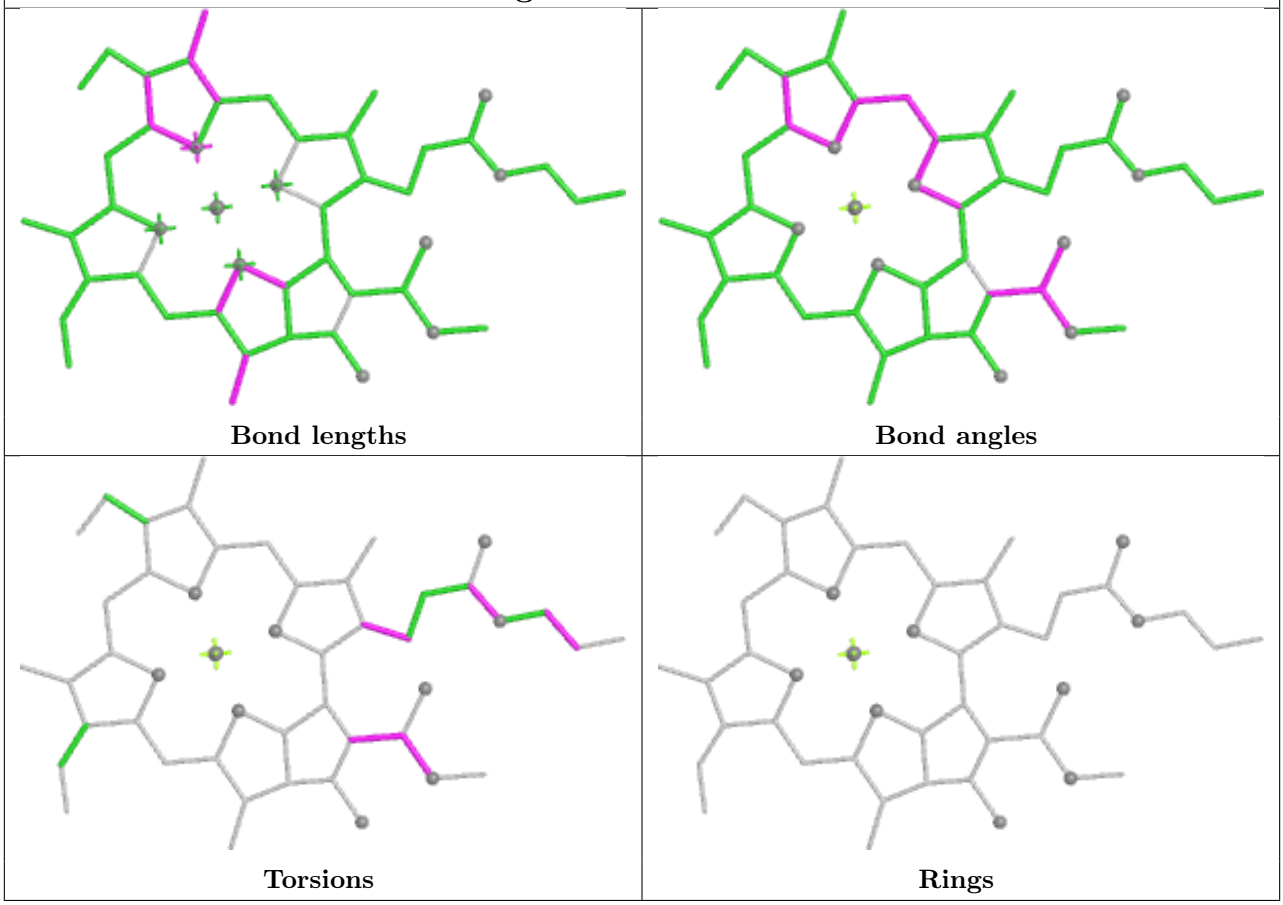


Rings

Ligand CHL N 607



Ligand CLA A2 614



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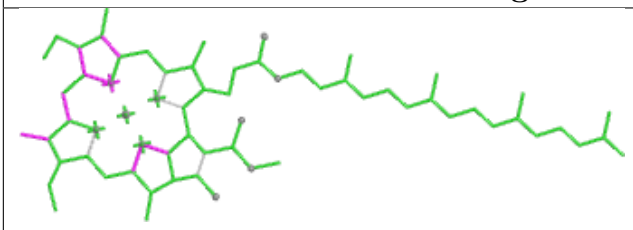

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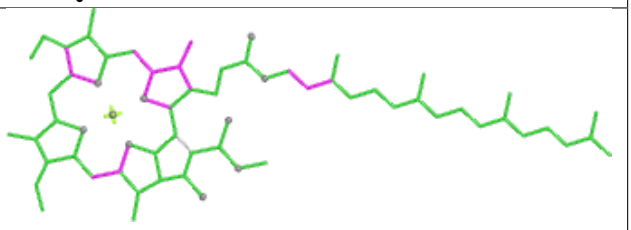
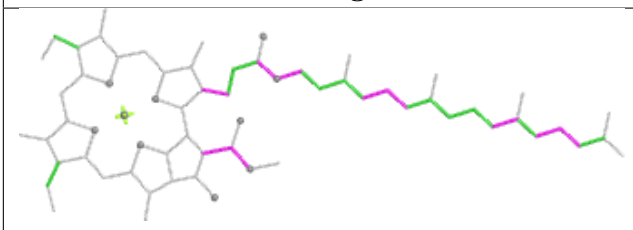


Bond angles



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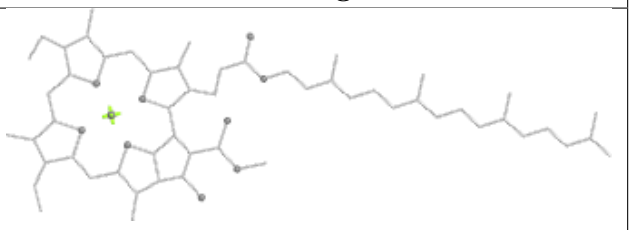

Rings

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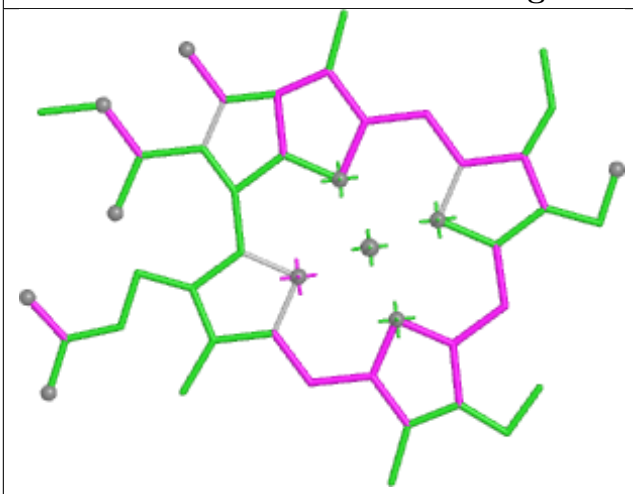

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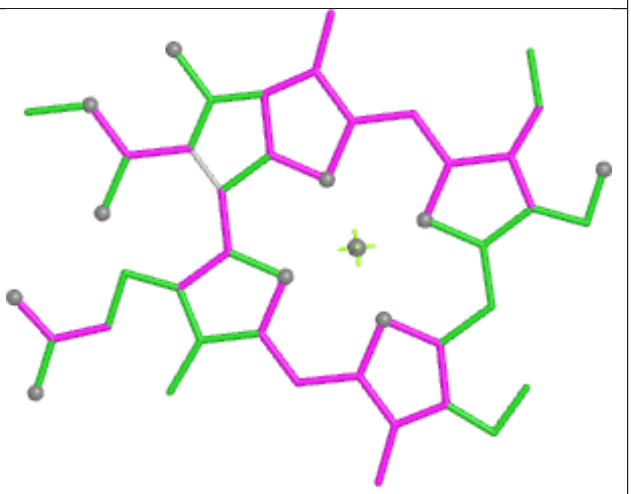
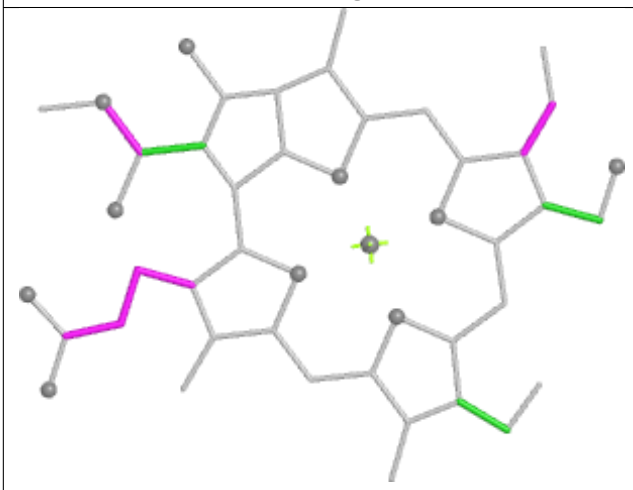


Bond angles



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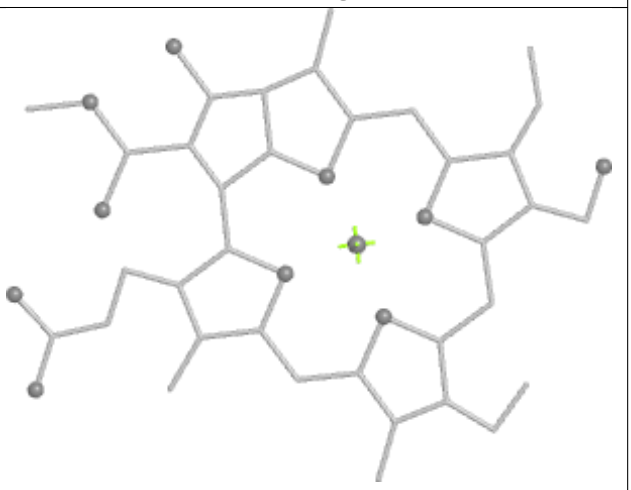
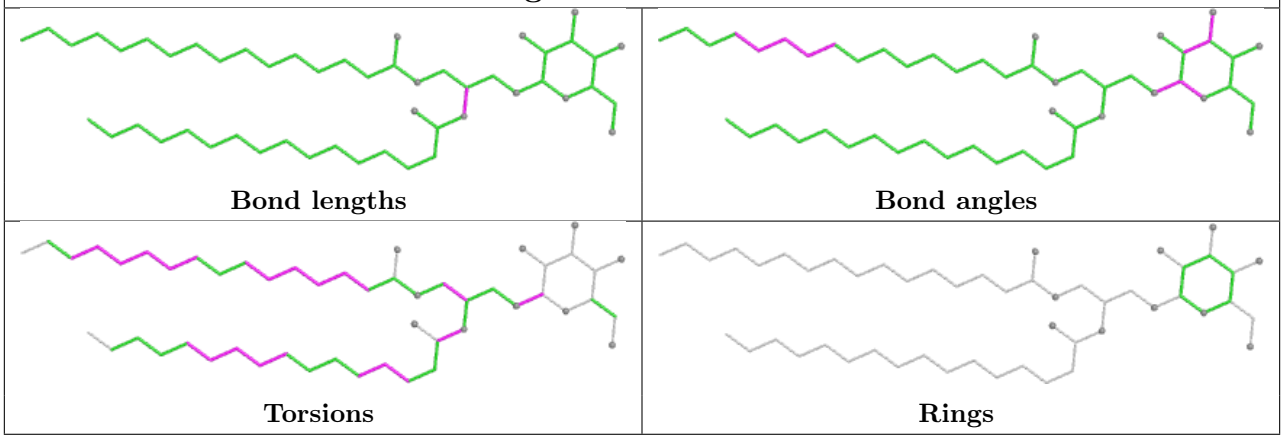
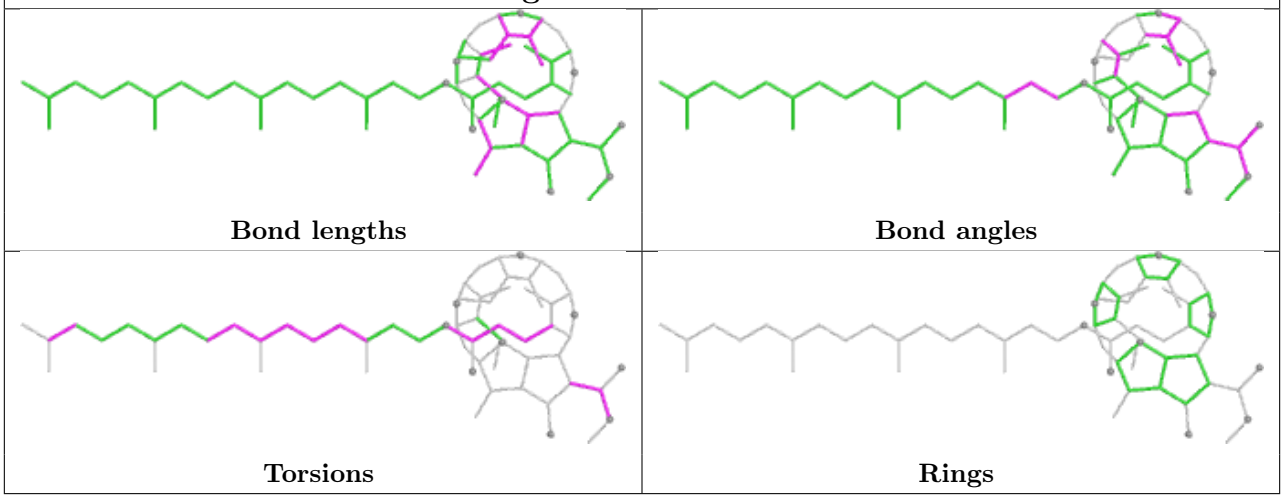


Rings

Ligand LMG 1 519



Ligand PHO A 409



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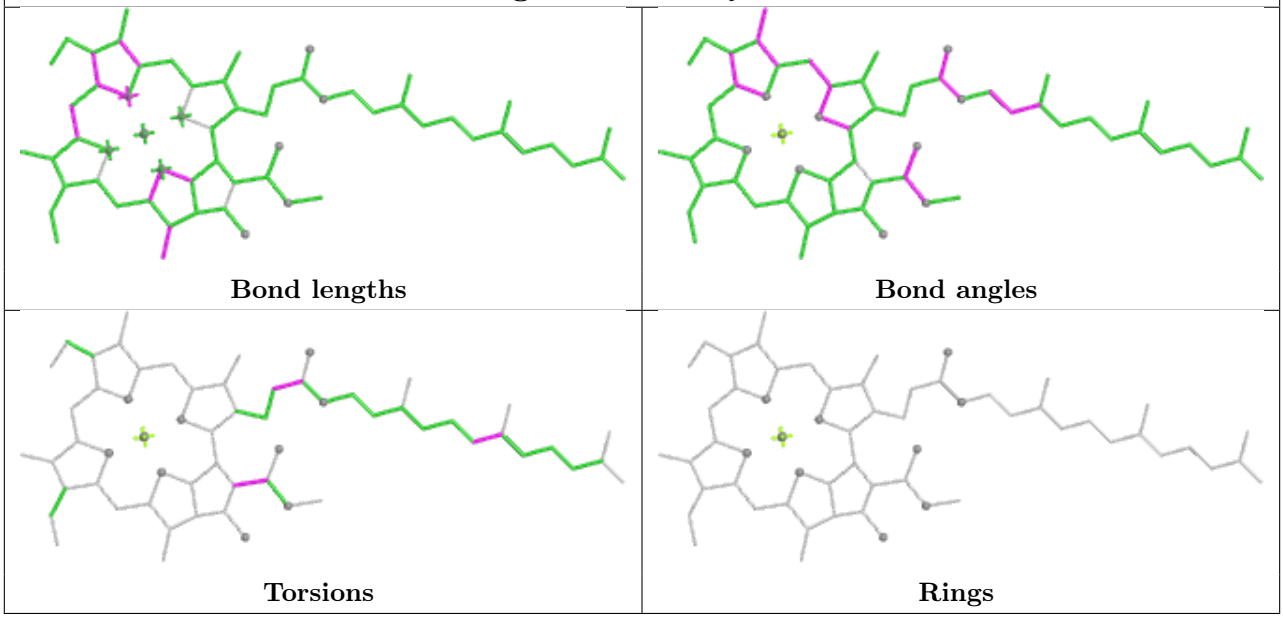

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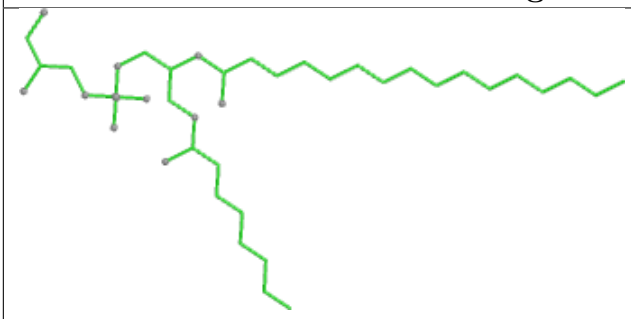
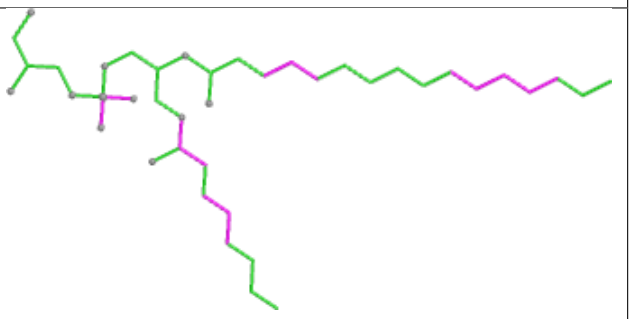
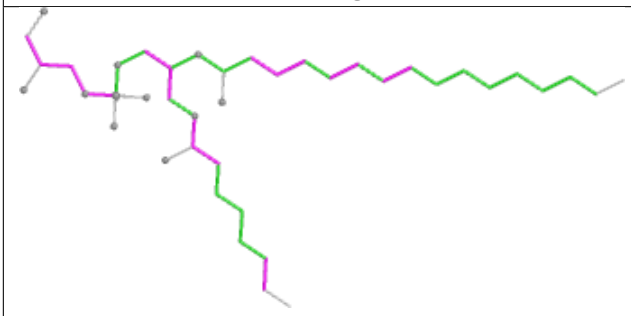
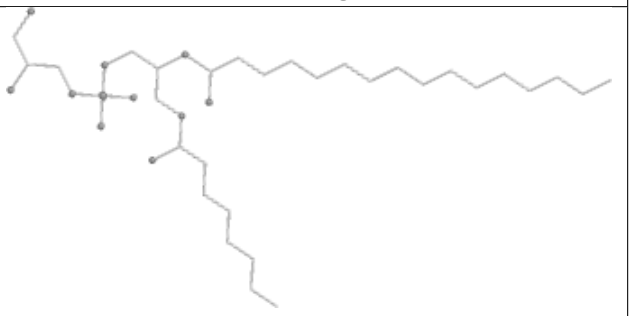
 Bond lengths	 Bond angles
 Torsions	 Rings

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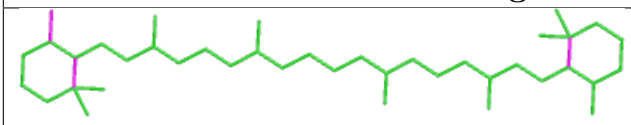
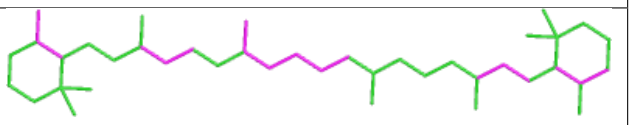
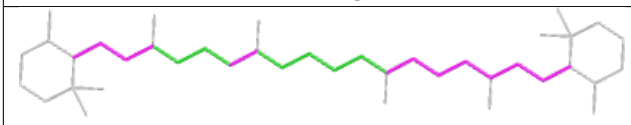
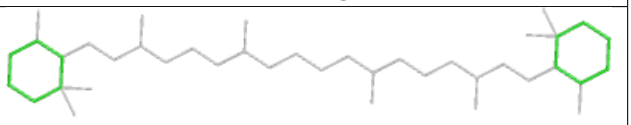
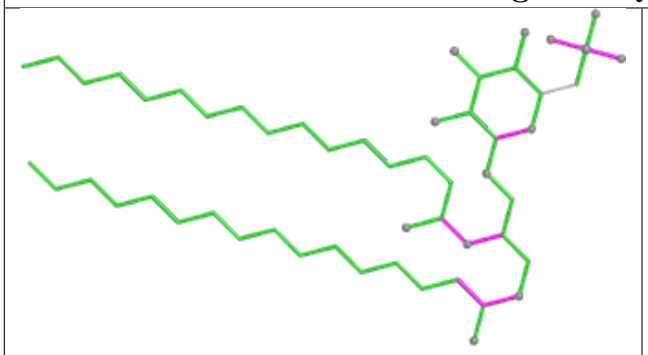
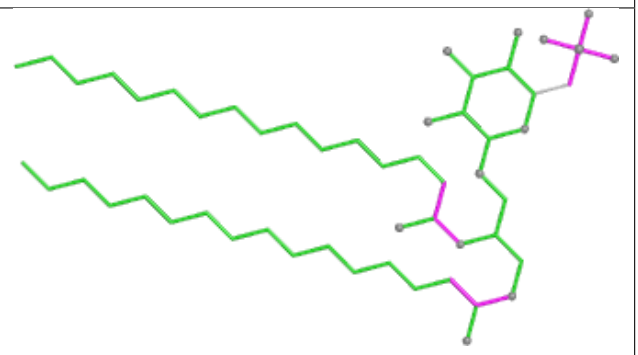
 Bond lengths	 Bond angles
 Torsions	 Rings

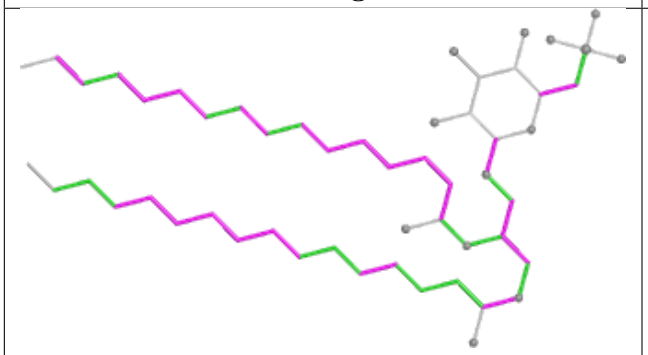
Ligand SQD BD 412



Bond lengths



Bond angles



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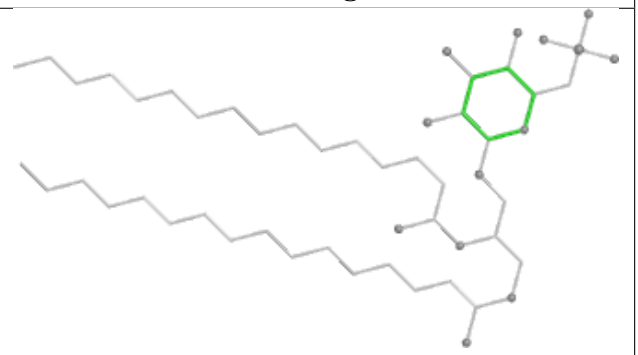
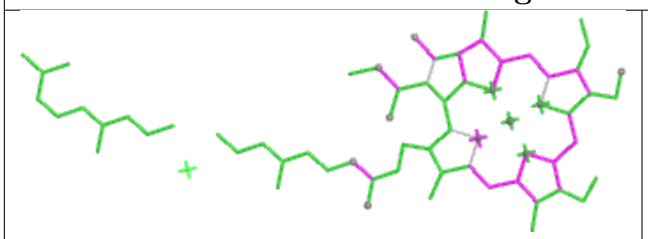


Rings

Ligand CHL Au 601



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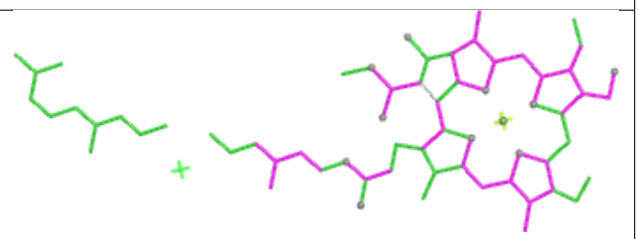
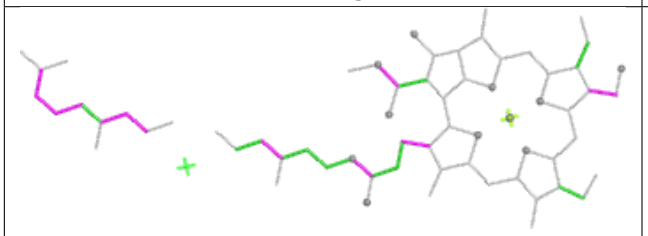


Bond angles



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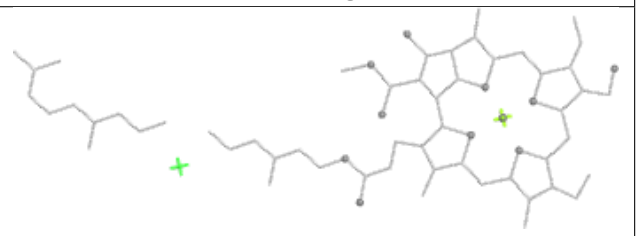
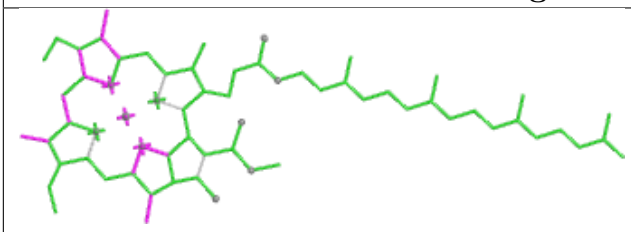


Rings

Ligand CLA c 507



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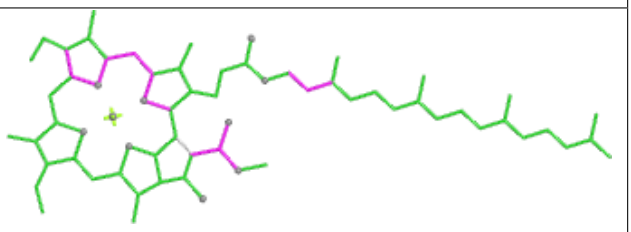

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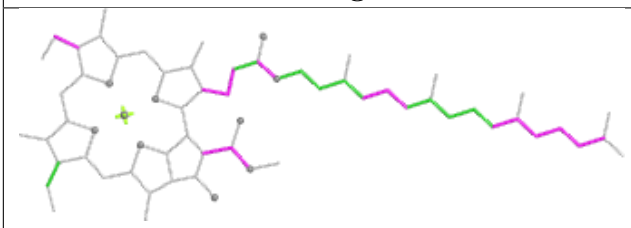

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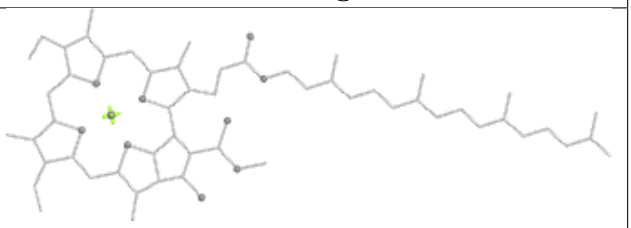
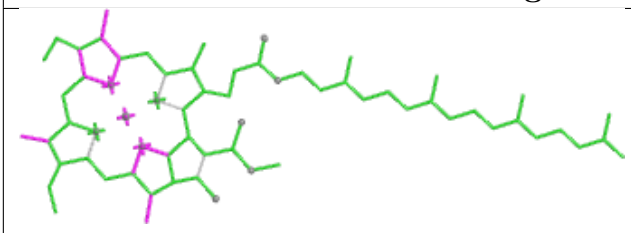


Rings

Ligand CLA C 508



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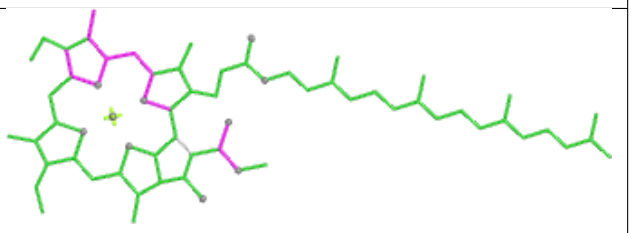

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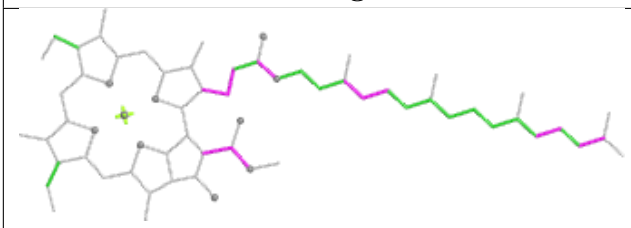

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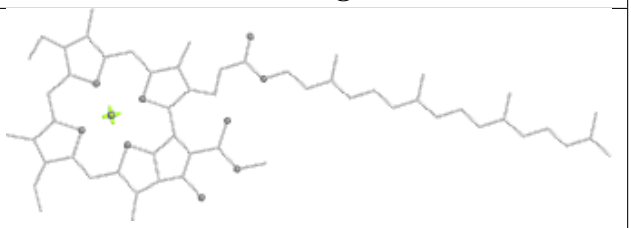
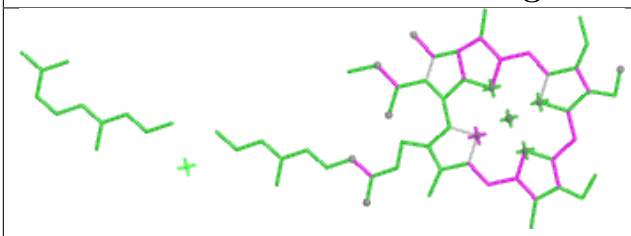


Rings

Ligand CHL Y 309



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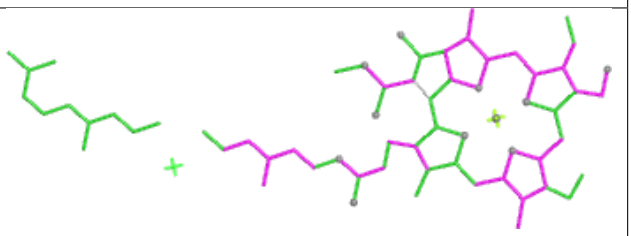

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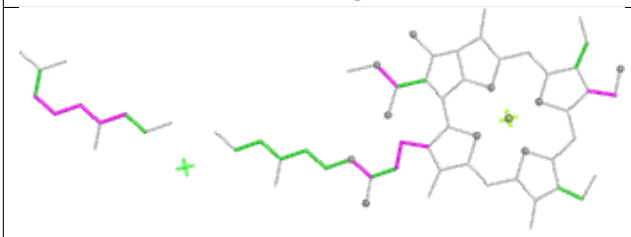

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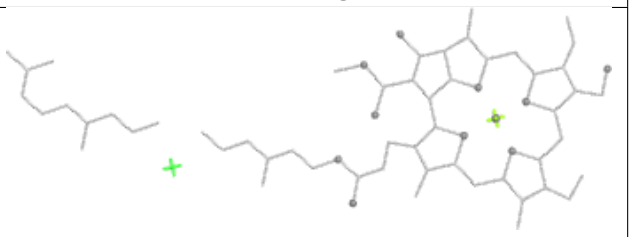
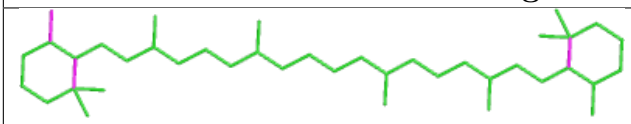


Rings

Ligand BCR R 410



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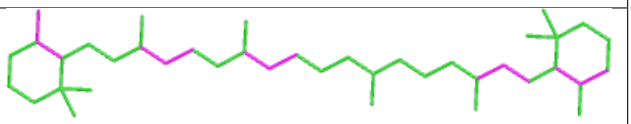
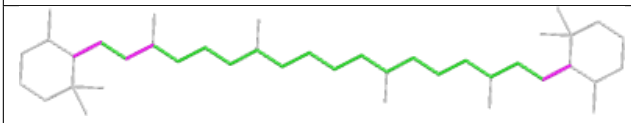
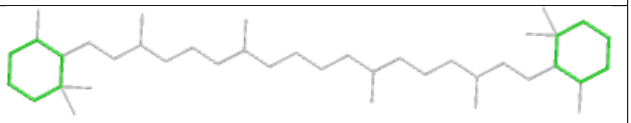


Bond angles

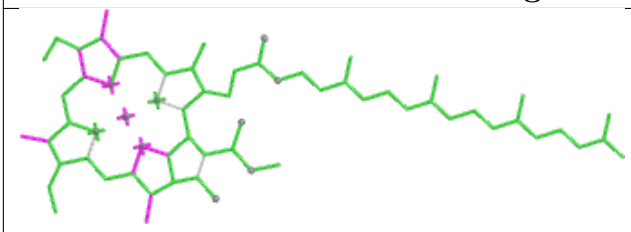


Torsions



Rings

Ligand CLA R 404



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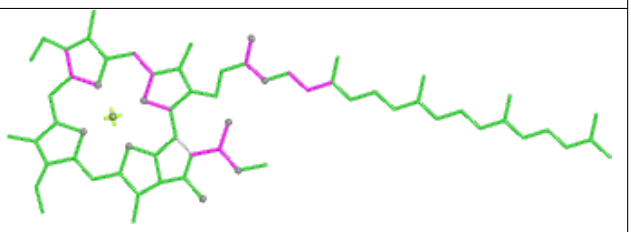
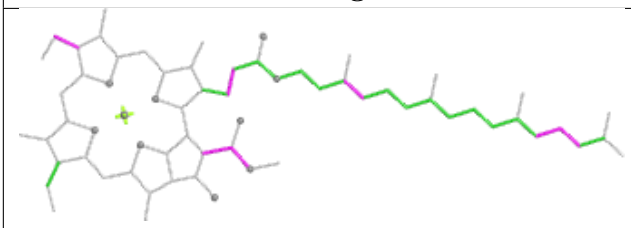
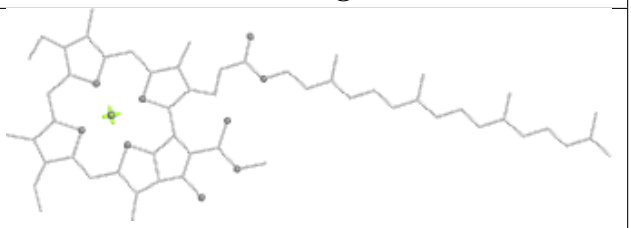


Bond angles

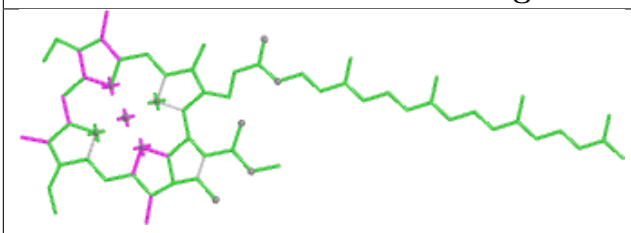


Torsions

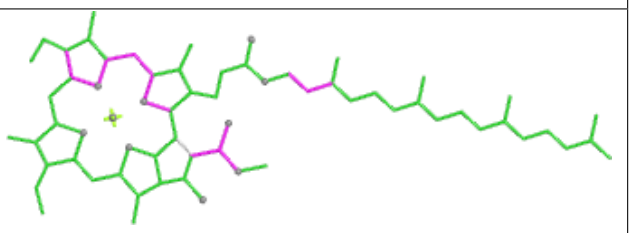


Rings

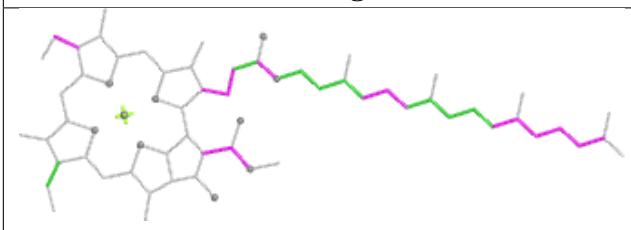
Ligand CLA BF 507



Bond lengths



Bond angles



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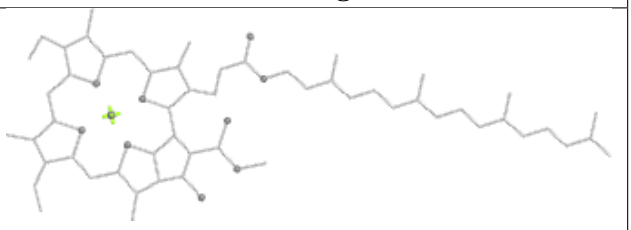
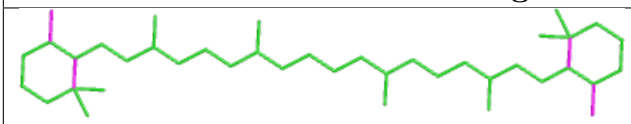


Rings

Ligand BCR BF 515



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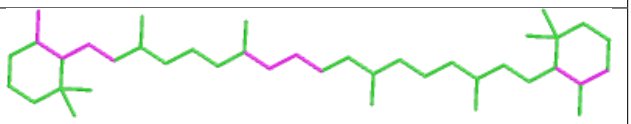

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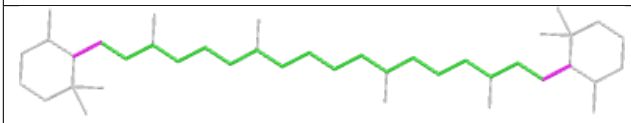

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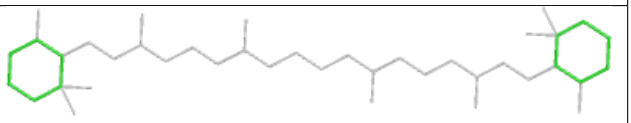
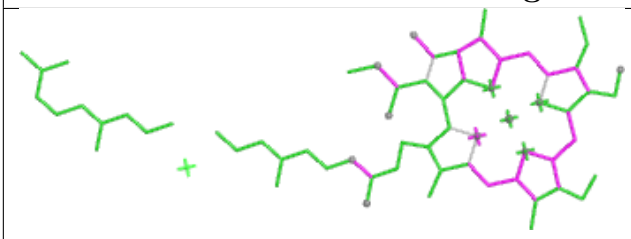


Rings

Ligand CHL Y 310



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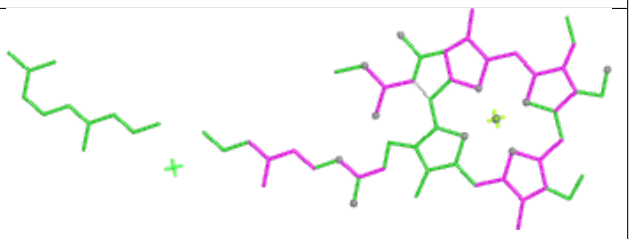

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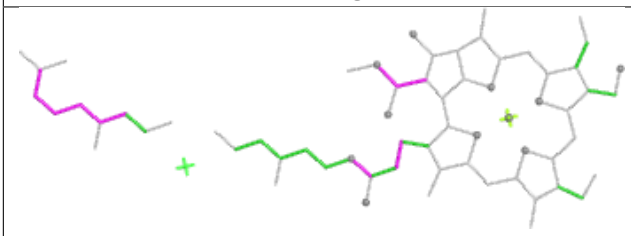

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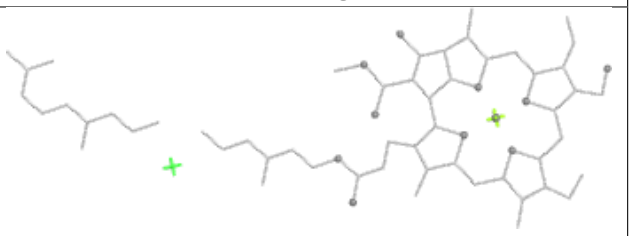
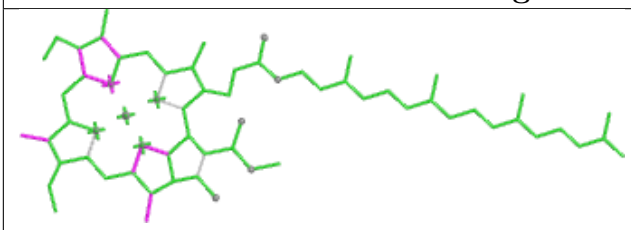


Rings

Ligand CLA BE 602



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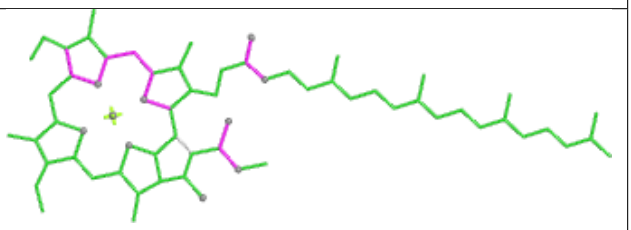
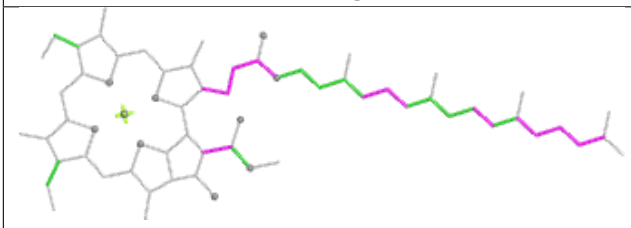


Bond angles



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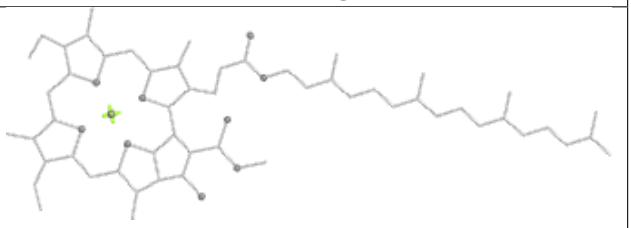
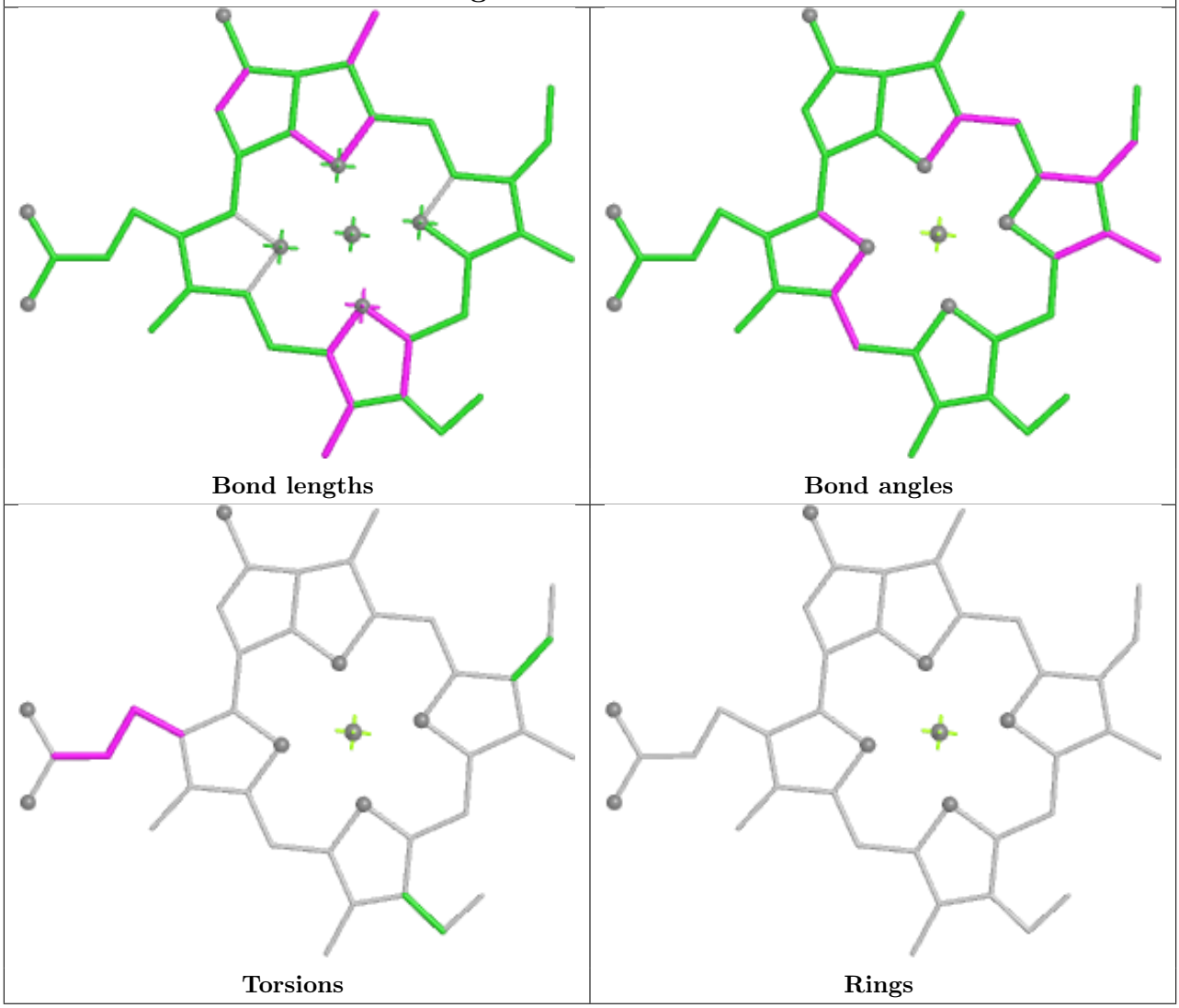
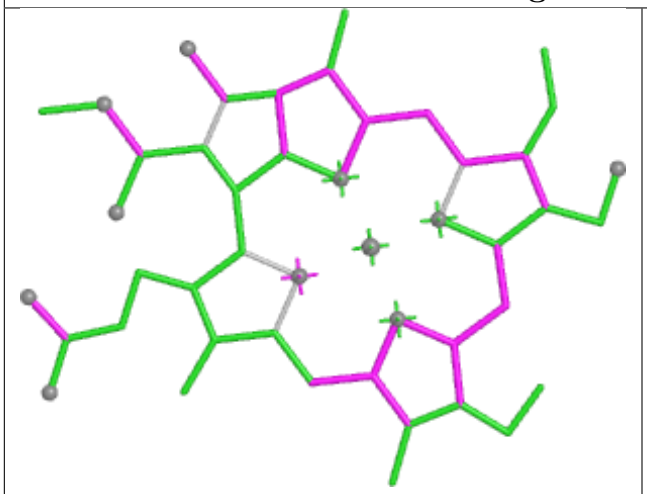


Rings

Ligand CLA AB 301



Ligand CHL 8 304



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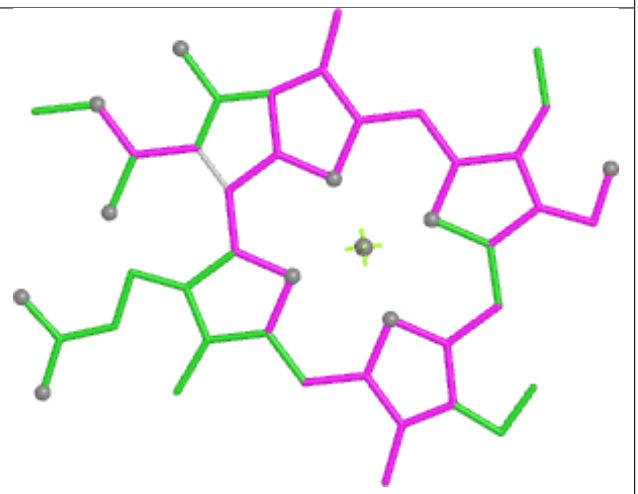

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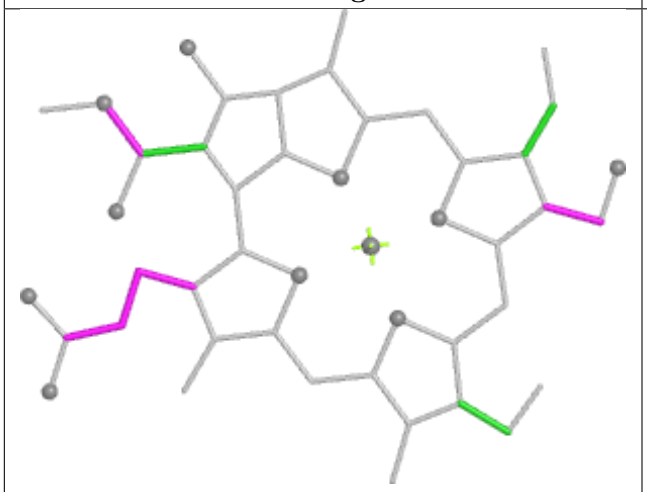

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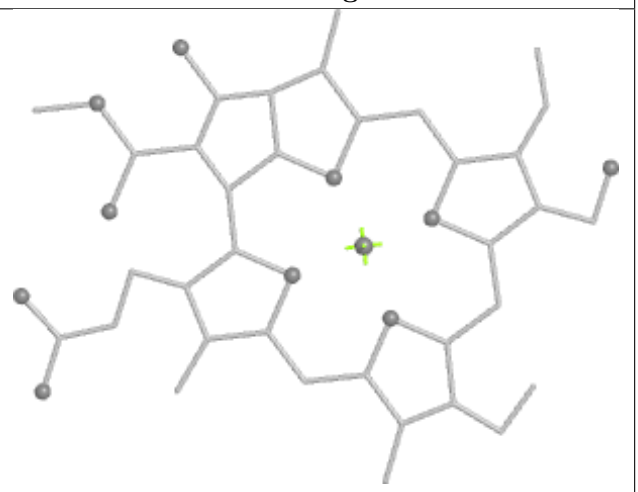

Rings

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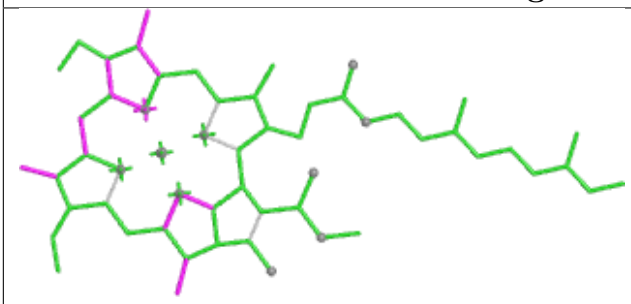
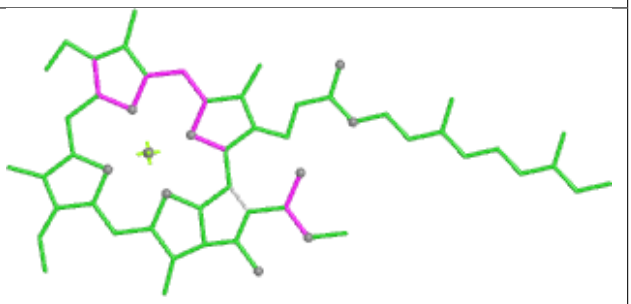
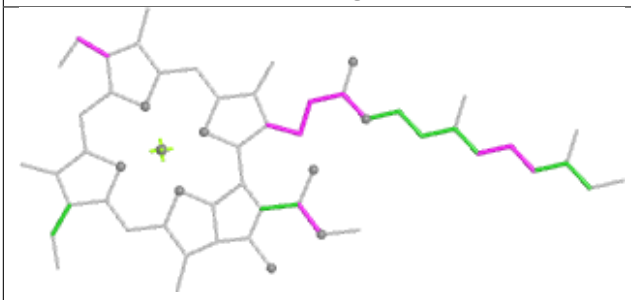
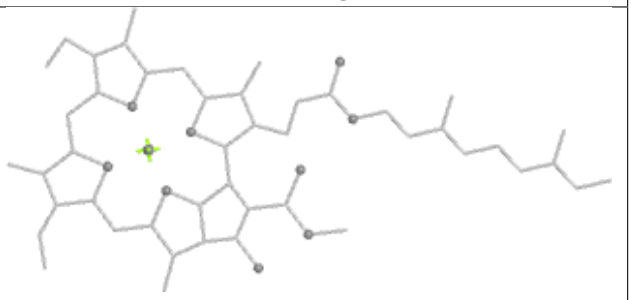
 Bond lengths	 Bond angles
 Torsions	 Rings

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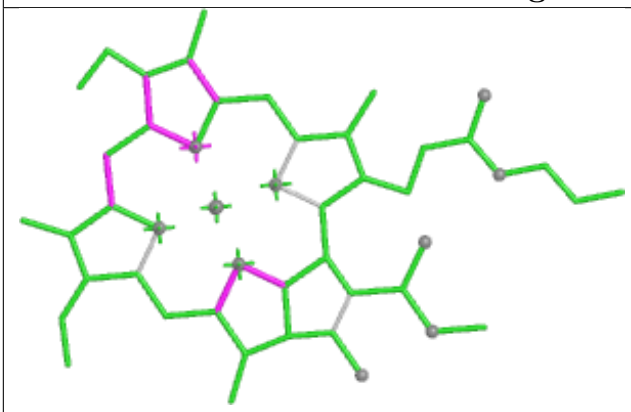
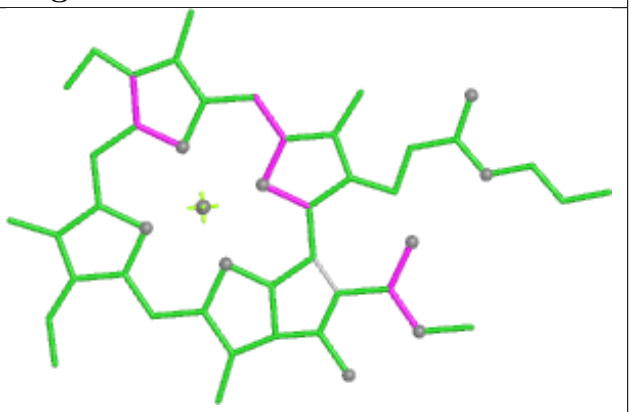
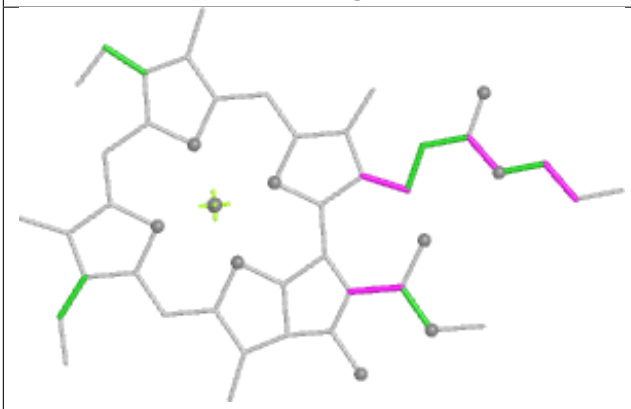
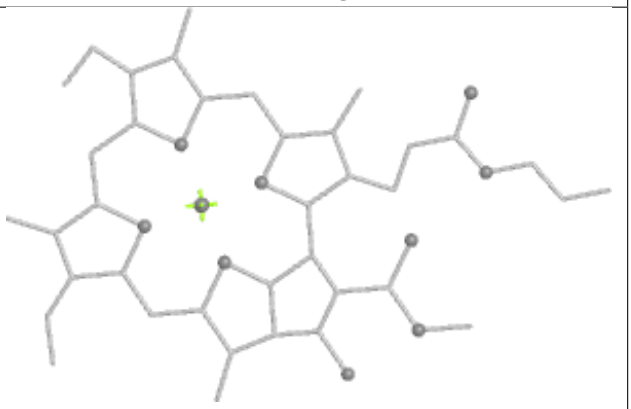
 Bond lengths	 Bond angles
 Torsions	 Rings

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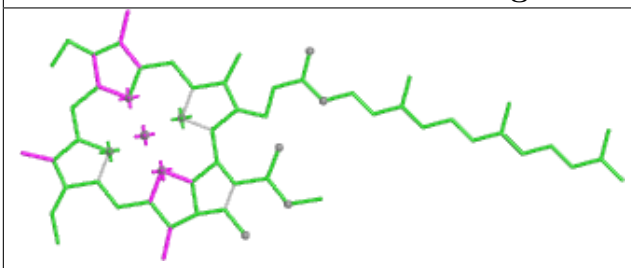
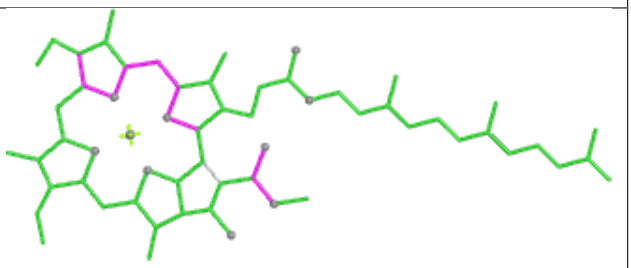
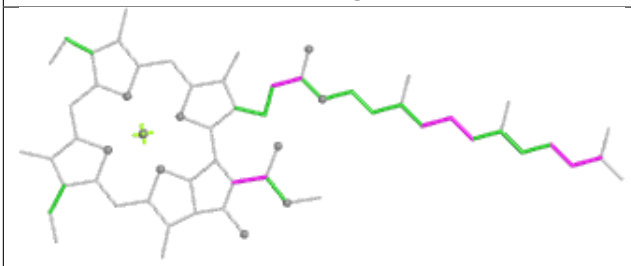
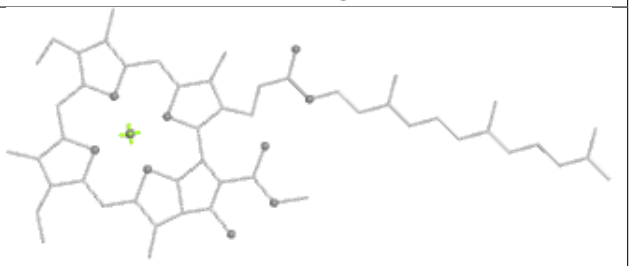
 Bond lengths	 Bond angles
 Torsions	 Rings

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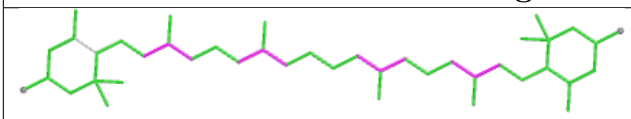
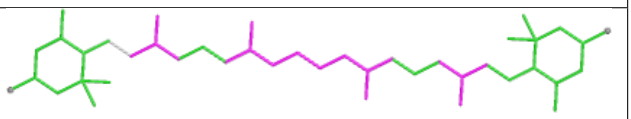
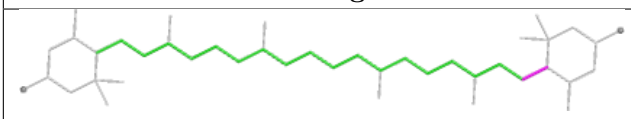
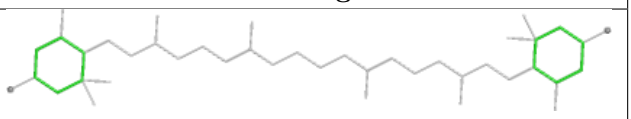
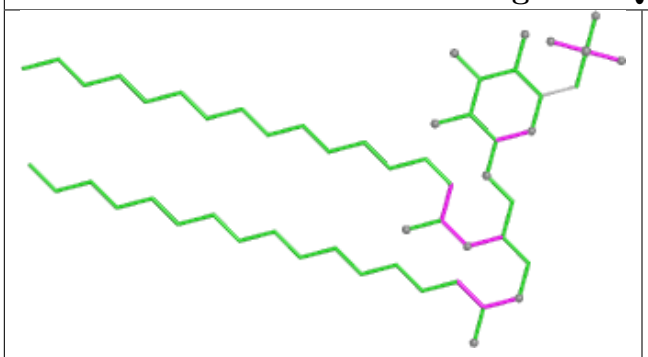
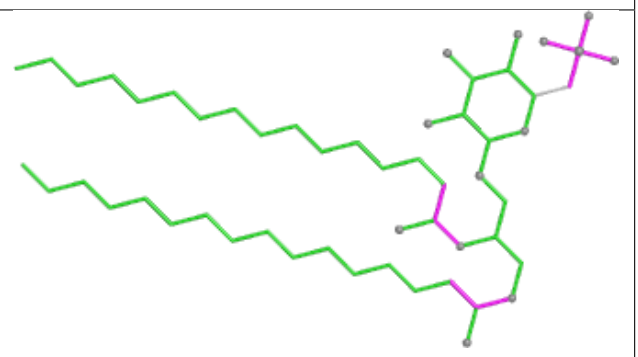
 Bond lengths	 Bond angles
 Torsions	 Rings

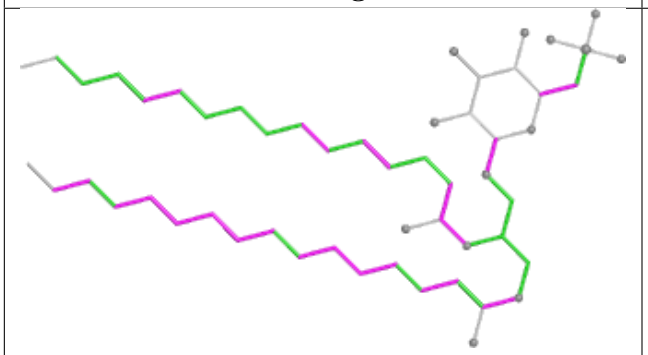
Ligand SQD BO 101



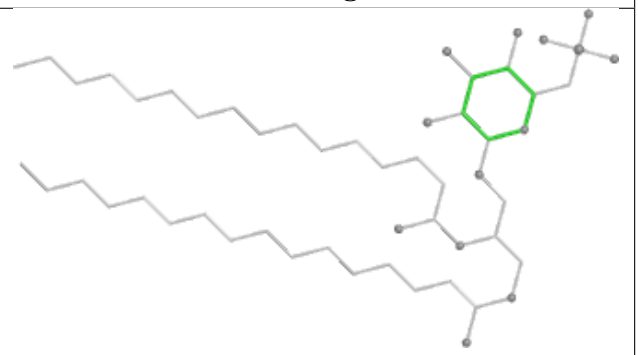
Bond lengths



Bond angles

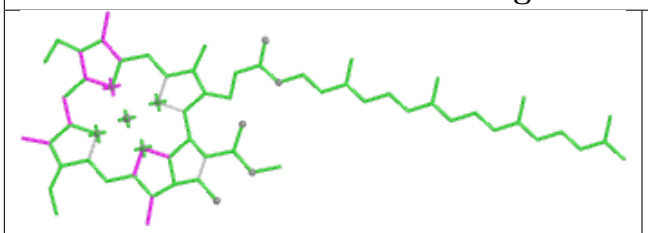


Torsions



Rings

Ligand CLA BE 615



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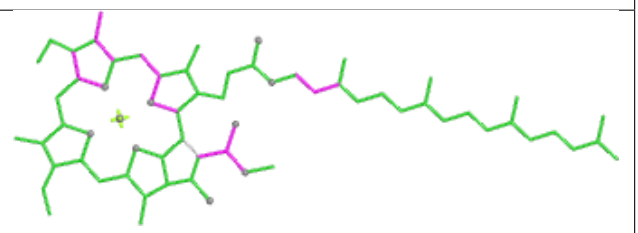
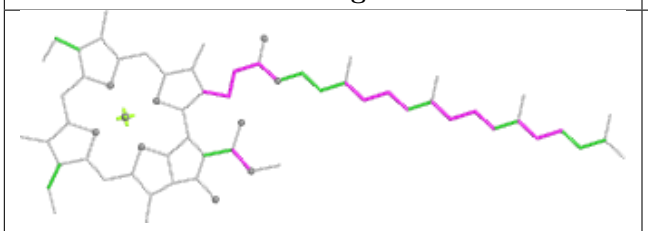


Bond angles



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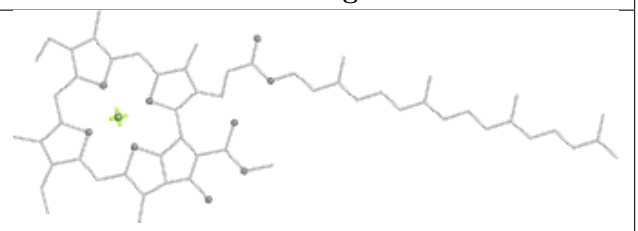
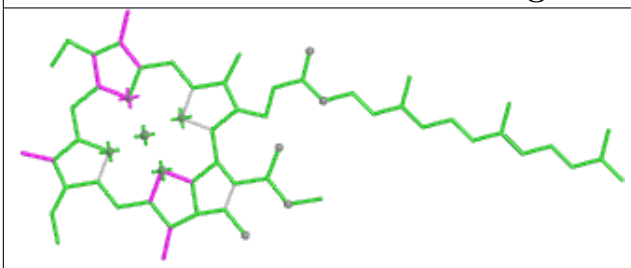
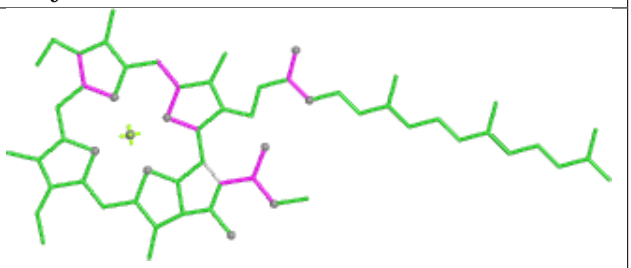
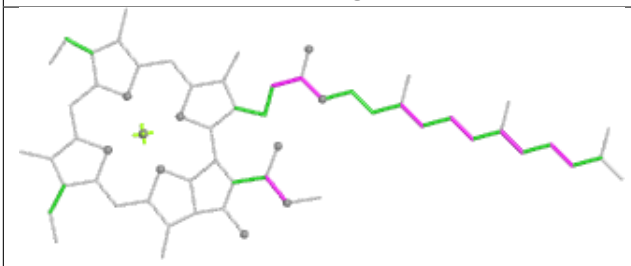
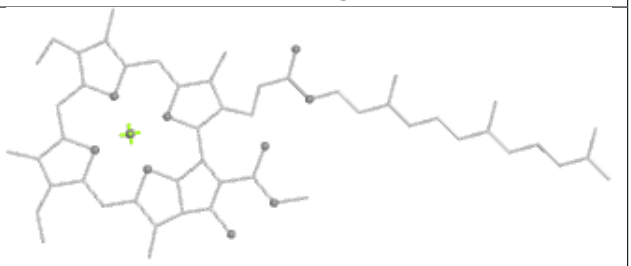


Rings

Ligand CLA y 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

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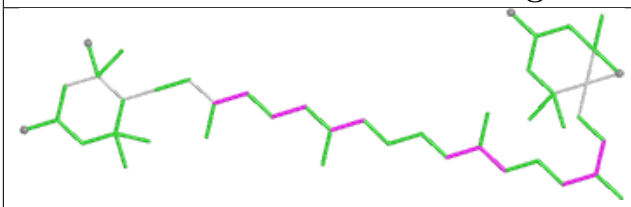
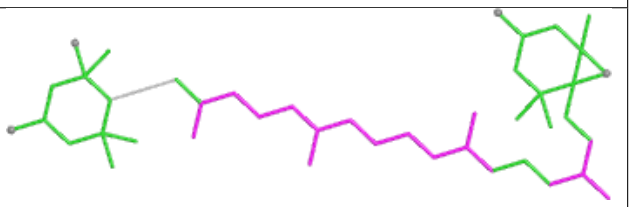
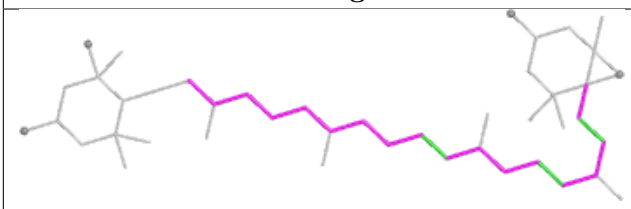
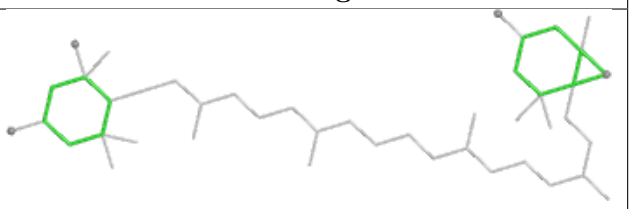
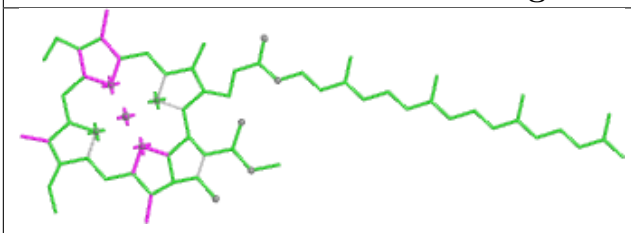
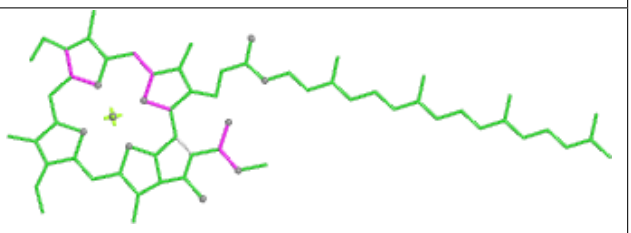
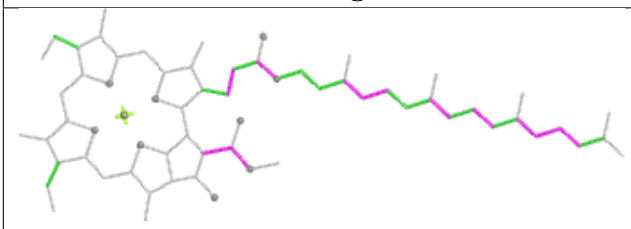
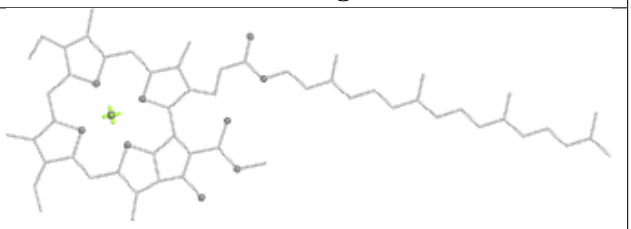
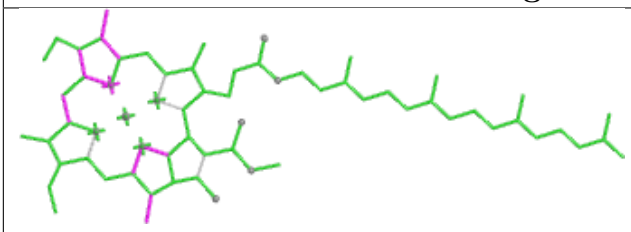
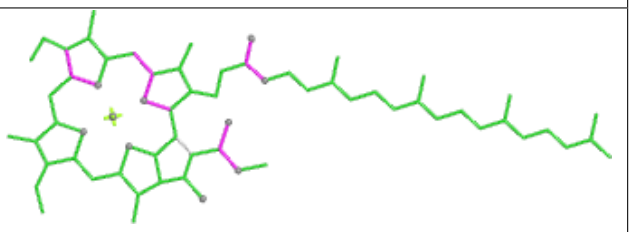
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

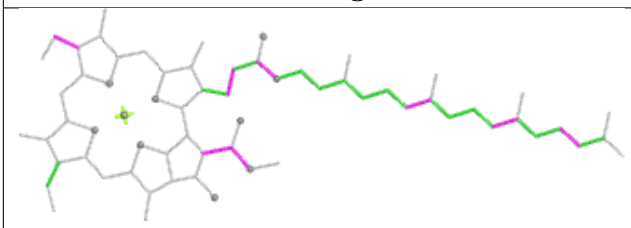
Ligand CLA D 402



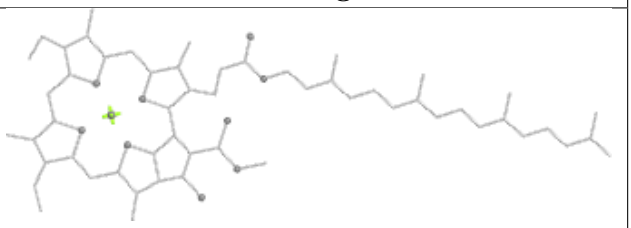
Bond lengths



Bond angles

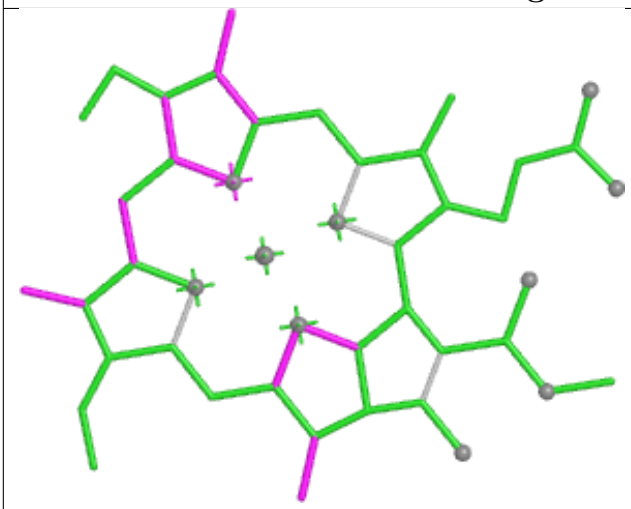


Torsions



Rings

Ligand CLA S 603



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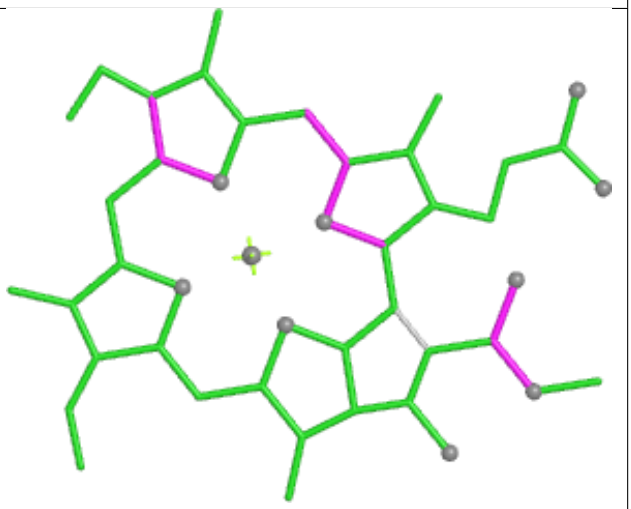

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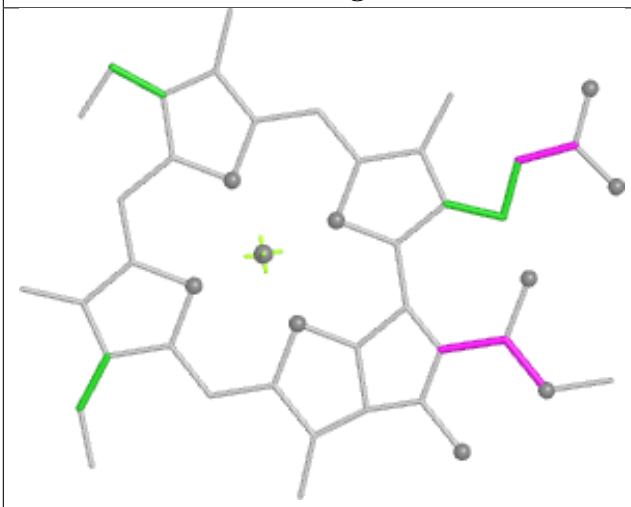

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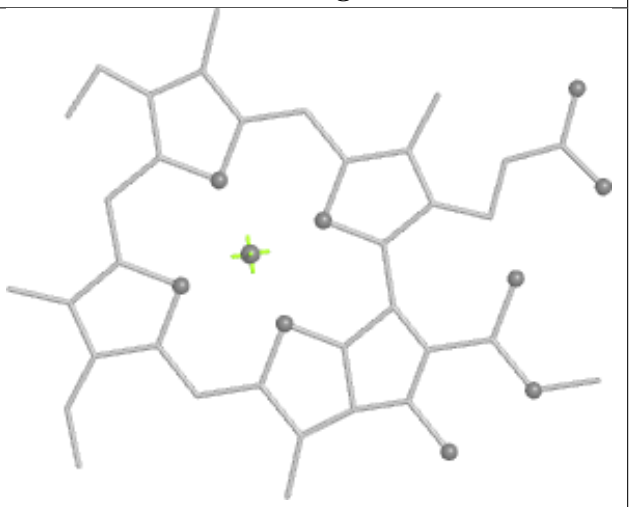
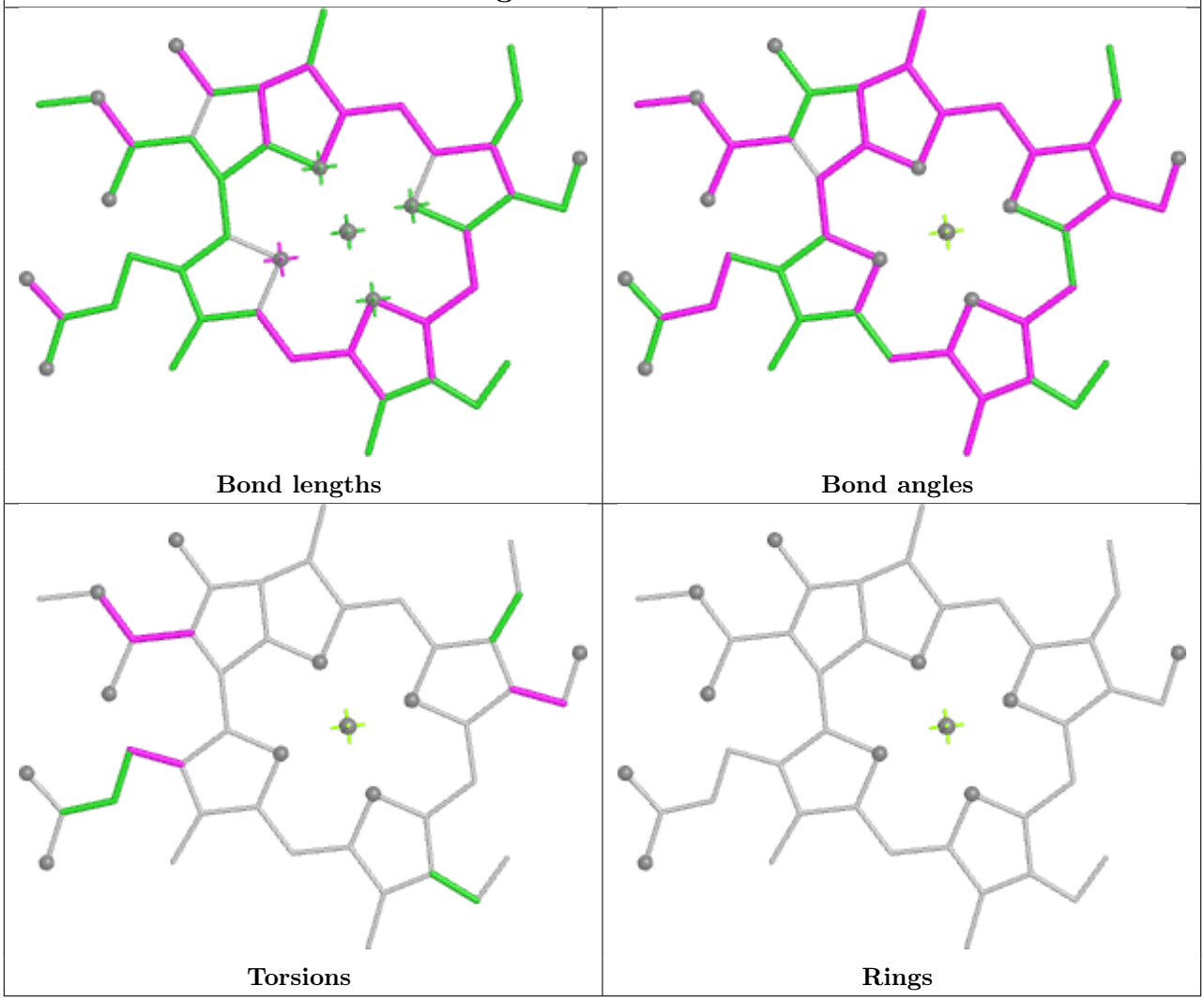
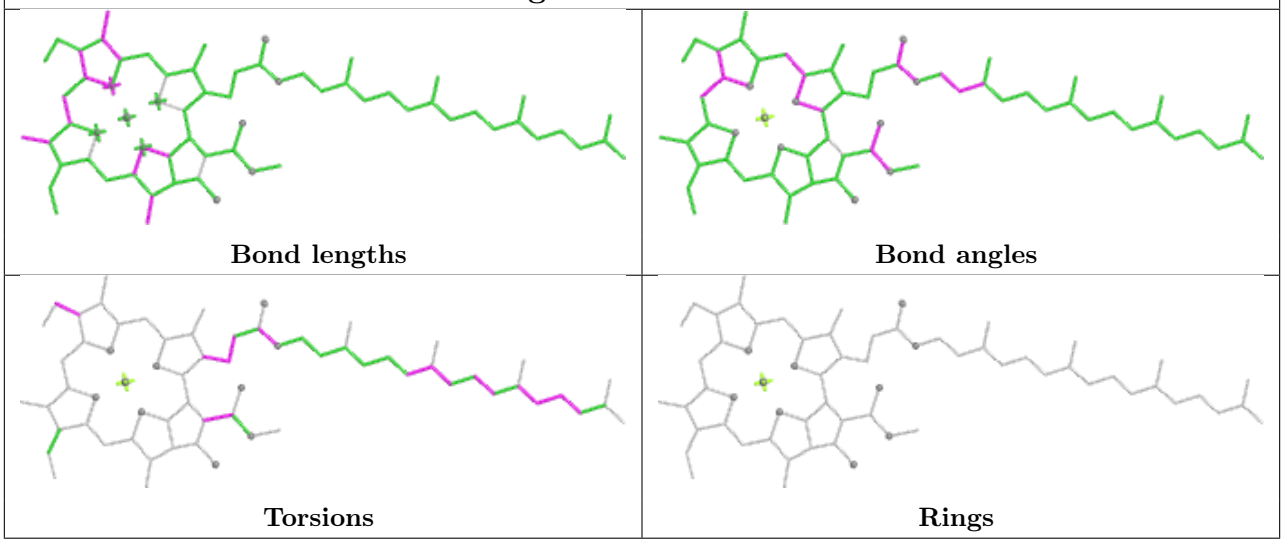


Rings

Ligand CHL 8 306



Ligand CLA b 613



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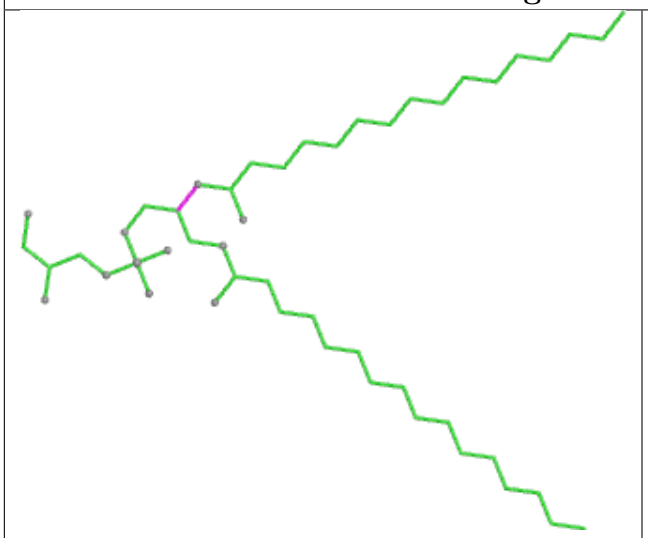

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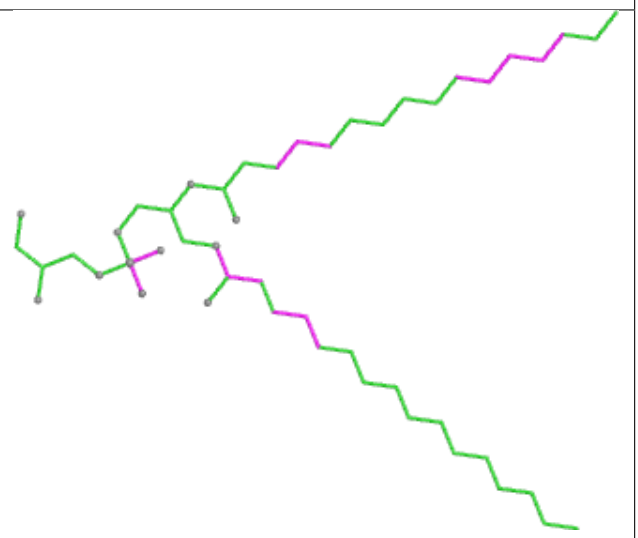

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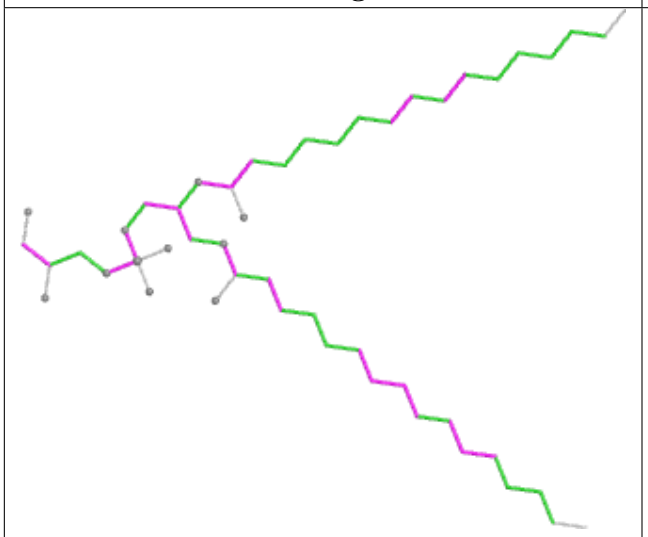

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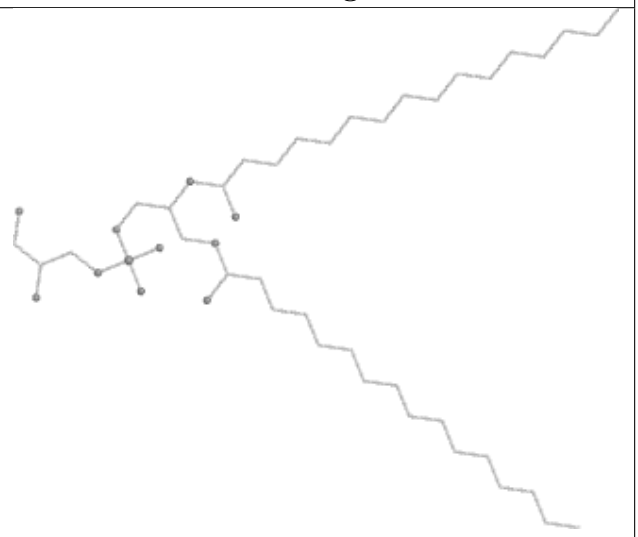
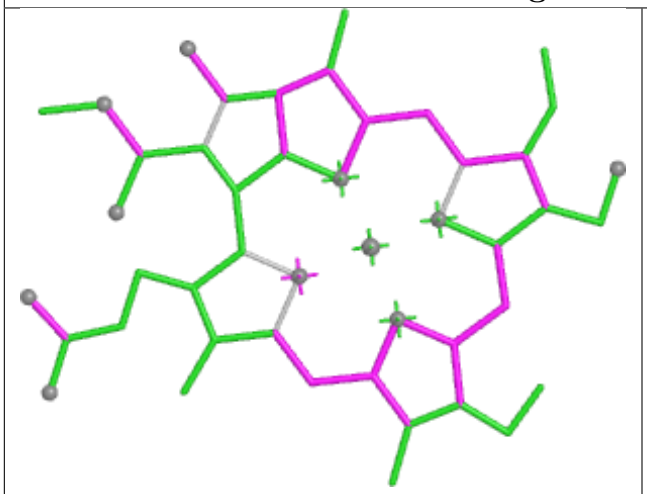


Rings

Ligand CHL 0 606



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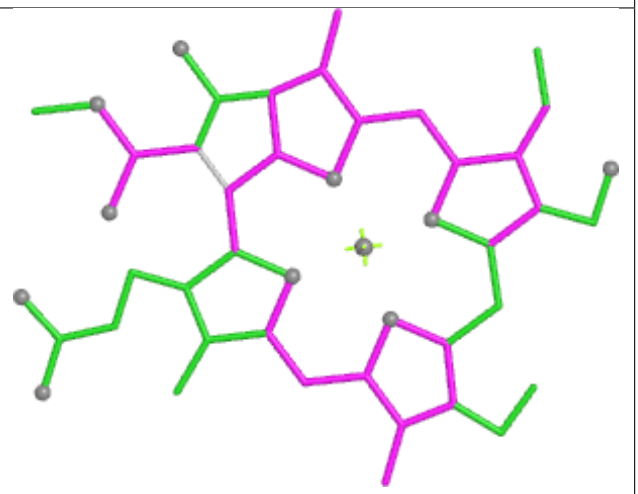

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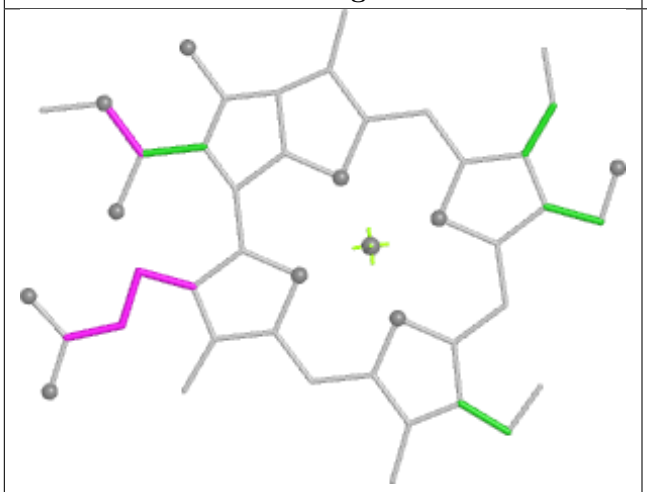

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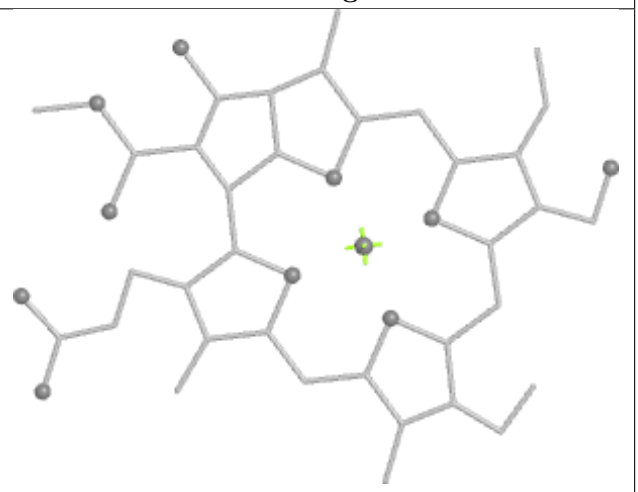
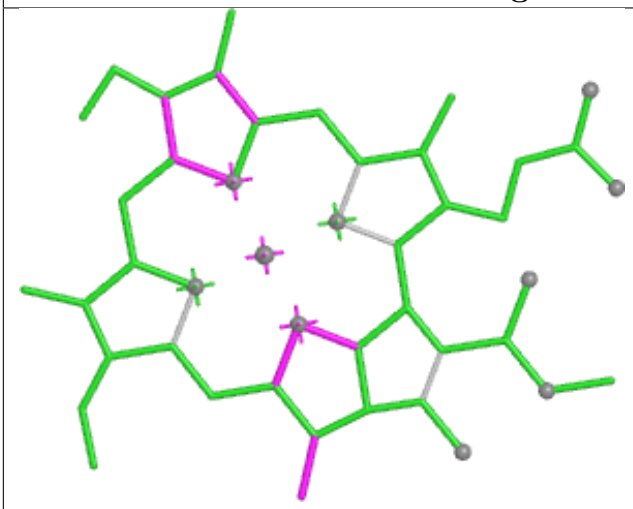


Rings

Ligand CLA AB 302



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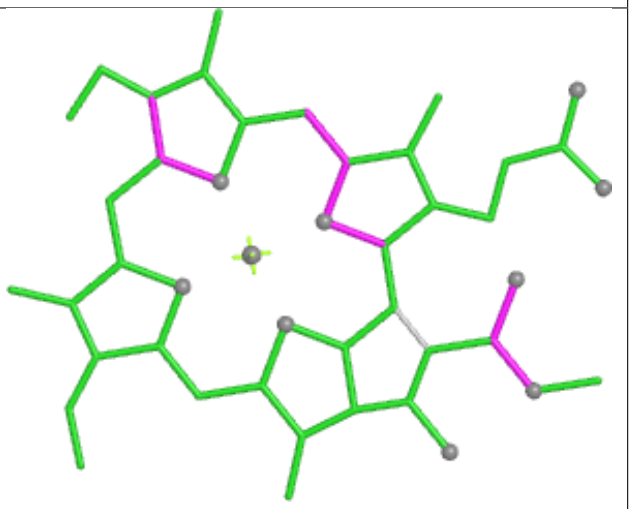

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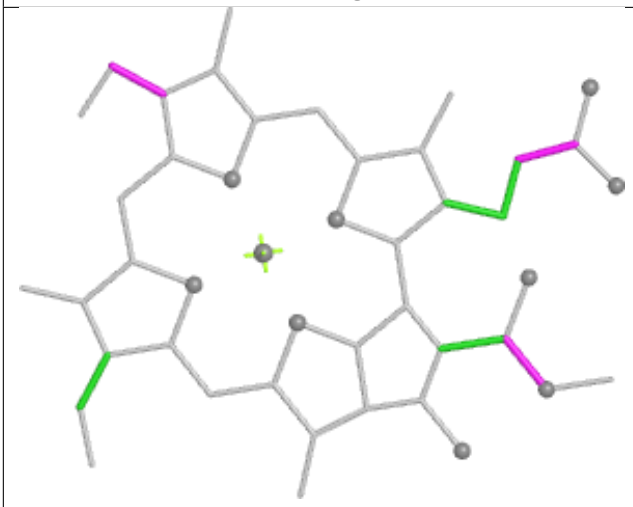
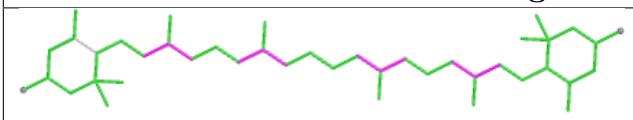


Torsions

Rings

Ligand LUT 5 616



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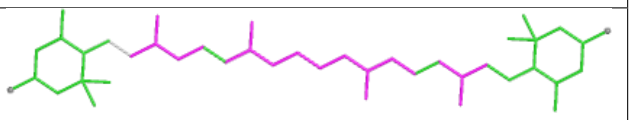
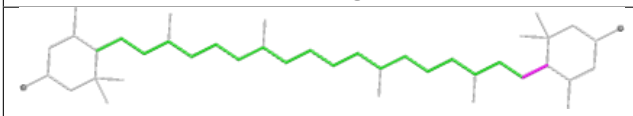


Bond angles



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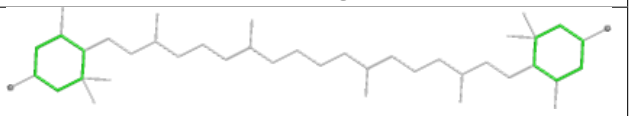
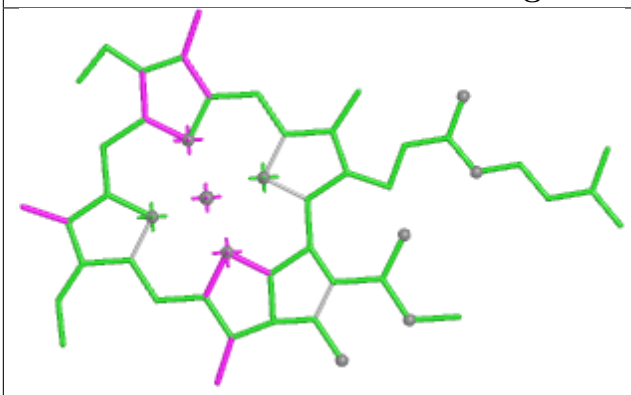
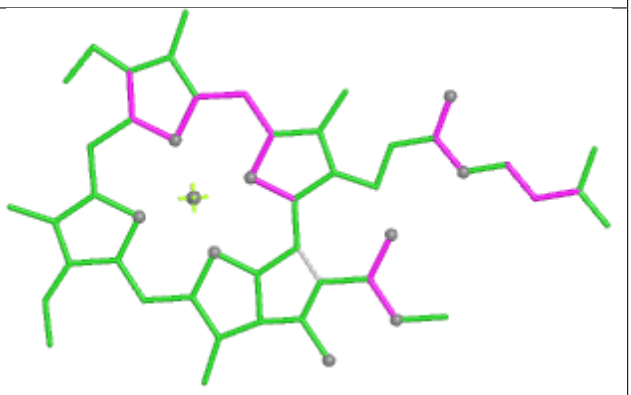
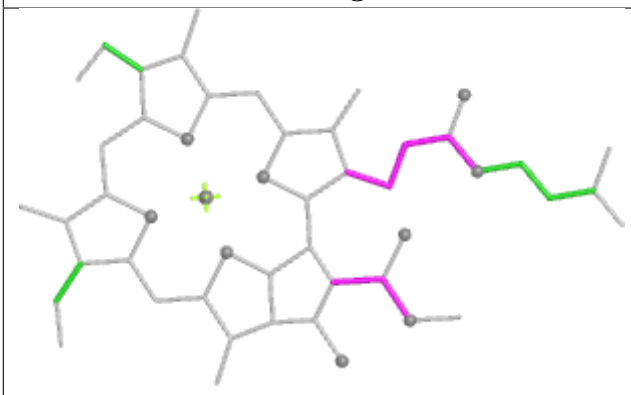
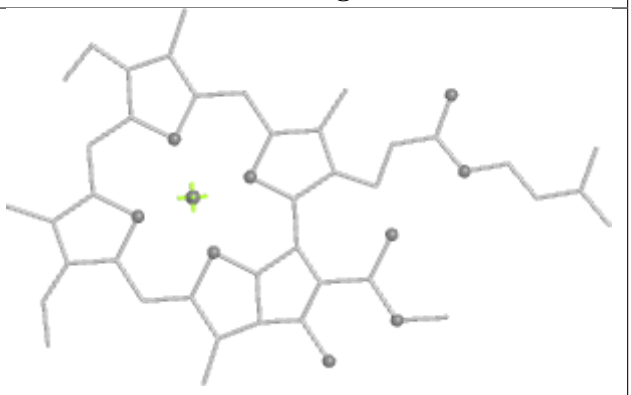
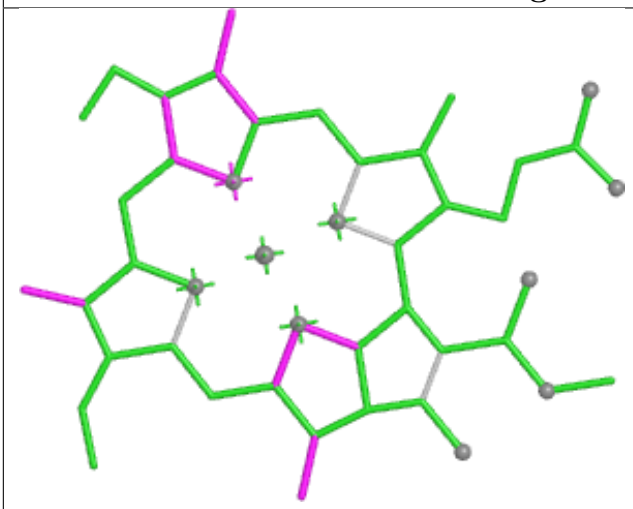


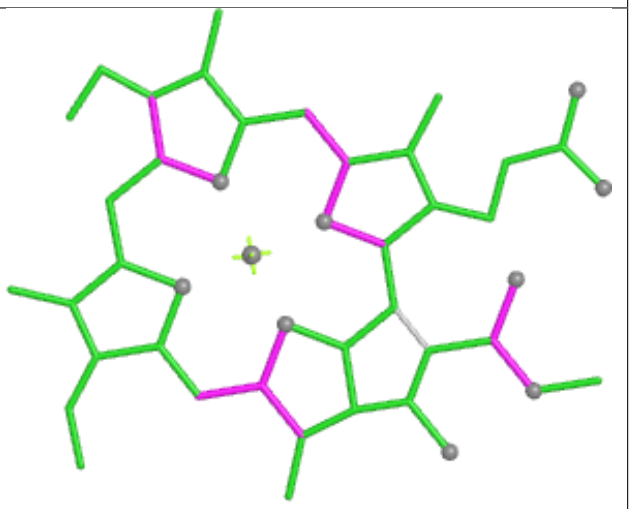
Rings

Ligand CLA Y 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

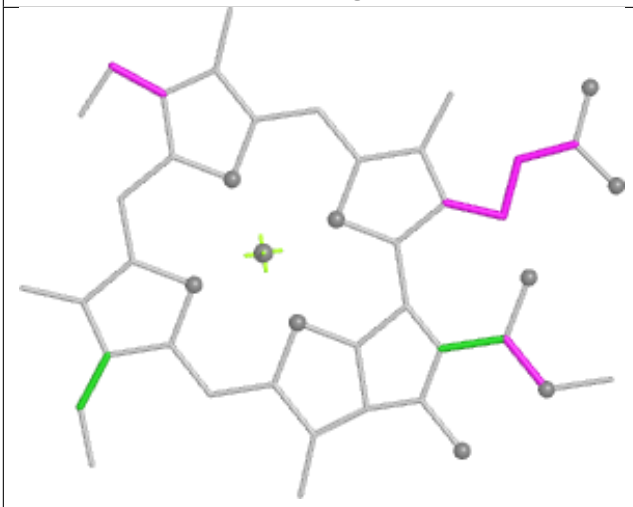
Ligand CLA r 614



Bond lengths



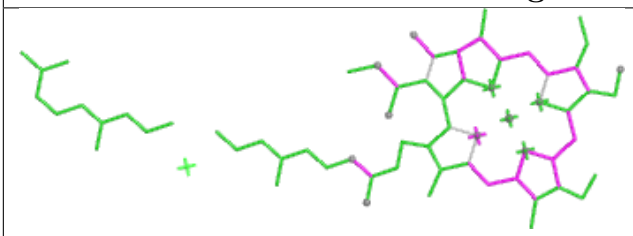
Bond angles



Torsions

Rings

Ligand CHL y 308



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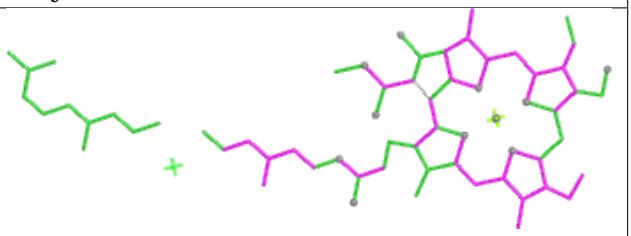
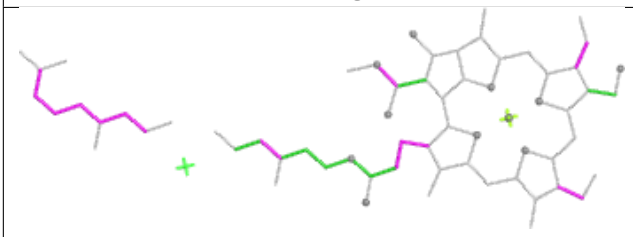
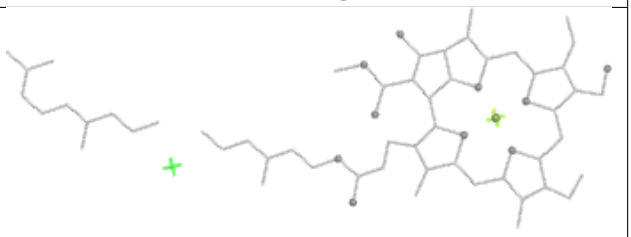


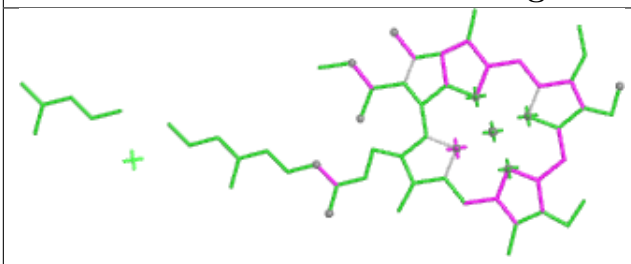
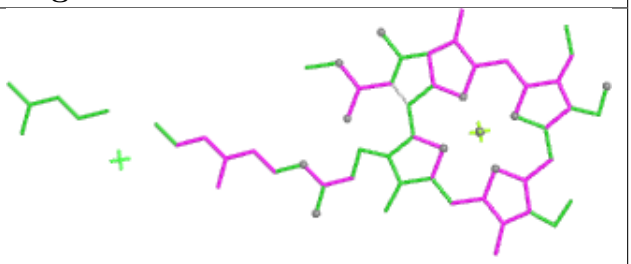
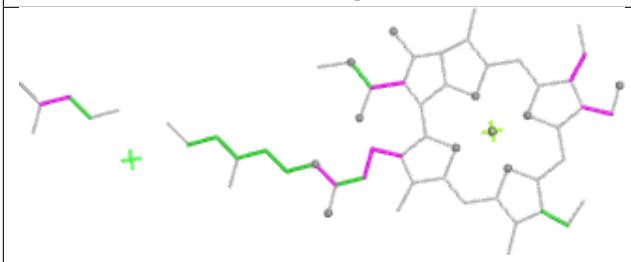
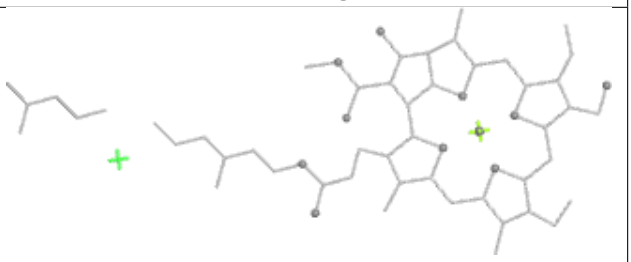
Bond angles

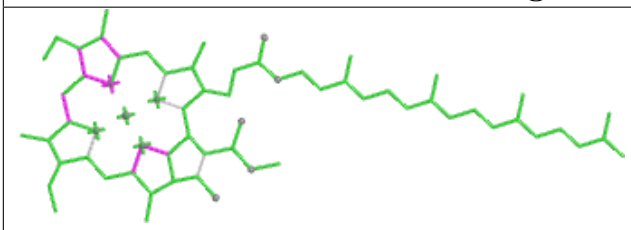
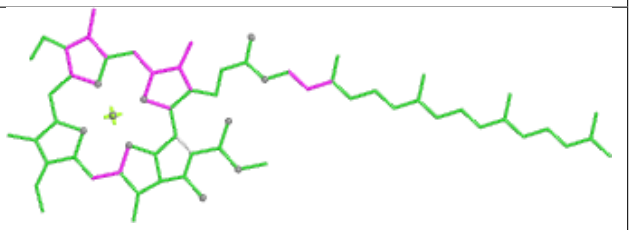
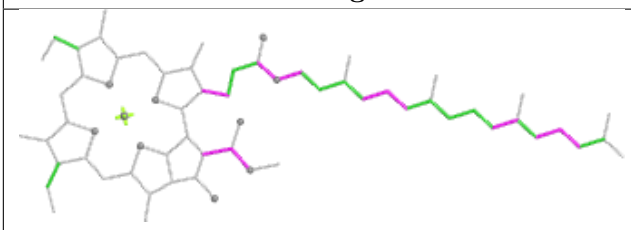
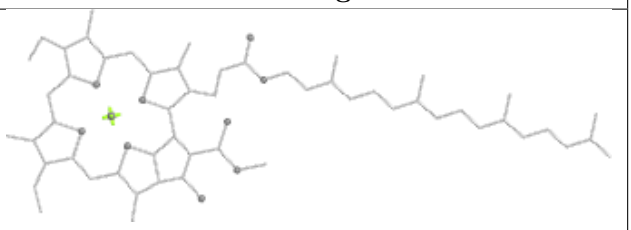


Torsions

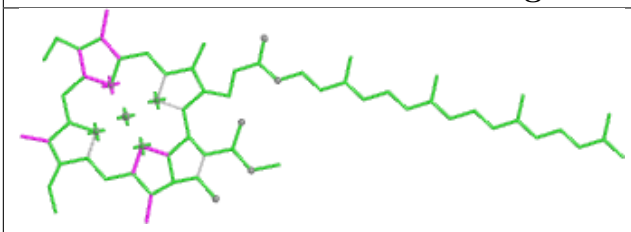


Rings

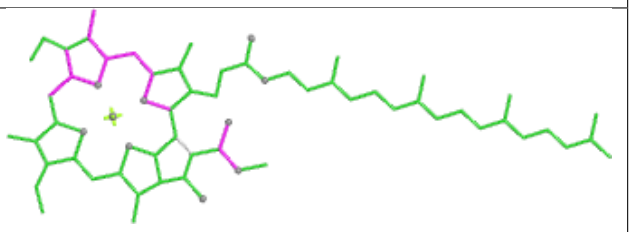
Ligand CHL g 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

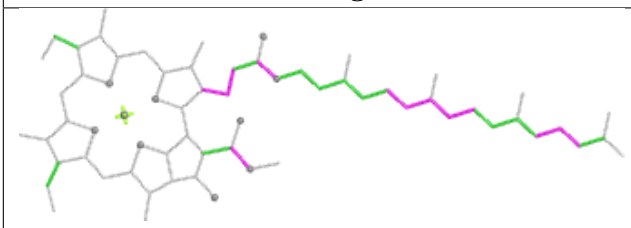
Ligand CLA B 608



Bond lengths



Bond angles



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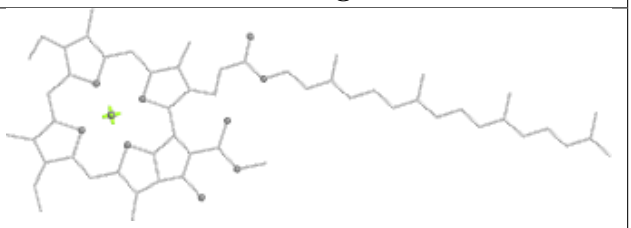
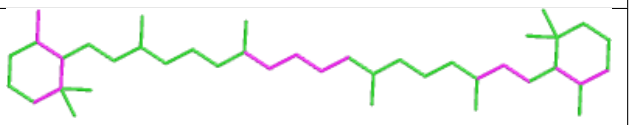


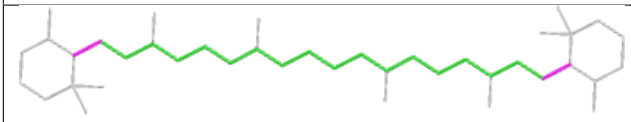
Rings

Ligand BCR 1 514

Bond lengths



Bond angles



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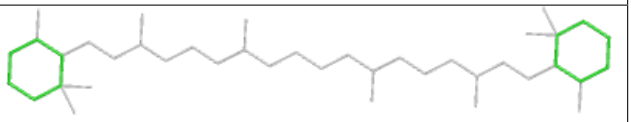
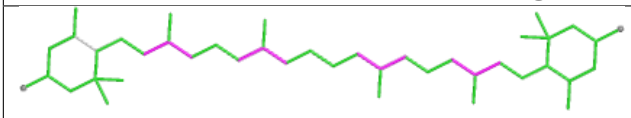
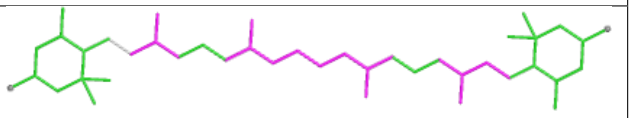


Rings

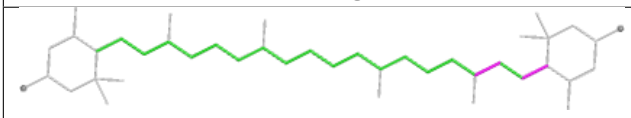
Ligand LUT r 615



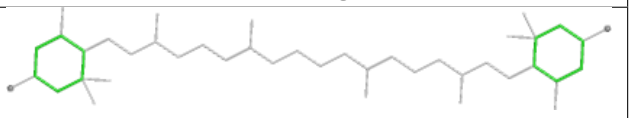
Bond lengths



Bond angles

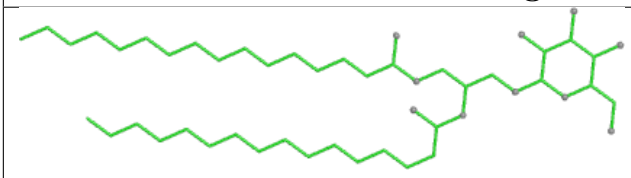


Torsions

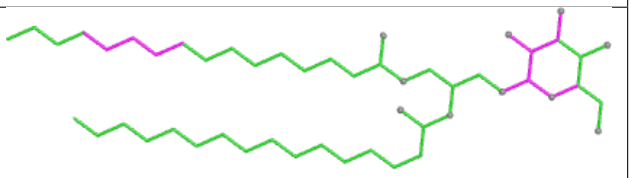


Rings

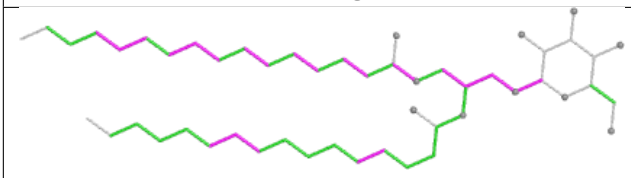
Ligand LMG 1 501



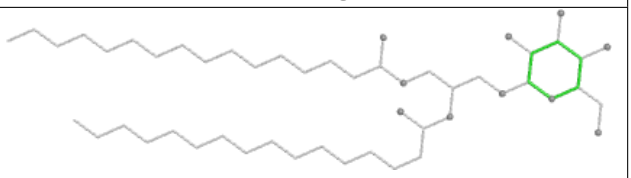
Bond lengths



Bond angles

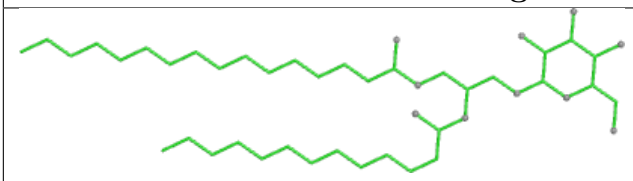


Torsions



Rings

Ligand LMG A0 201



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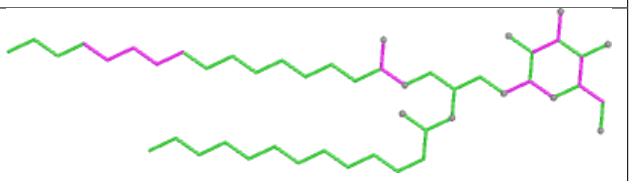
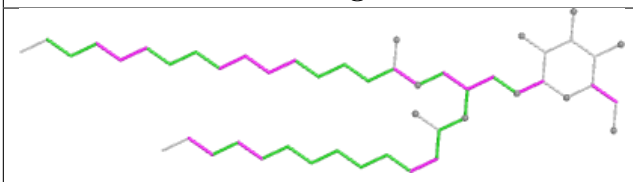


Bond angles



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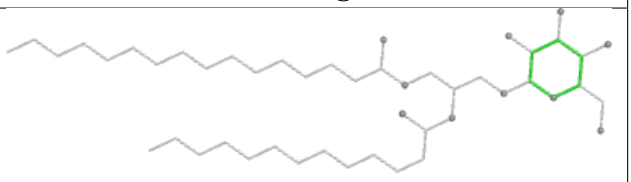
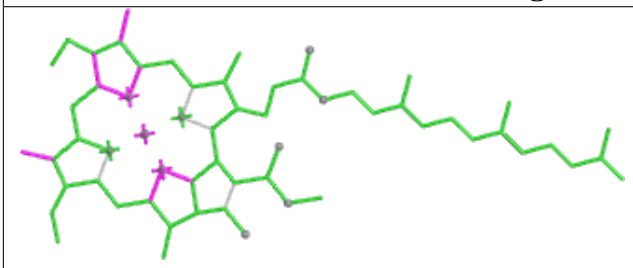


Rings

Ligand CLA 6 602



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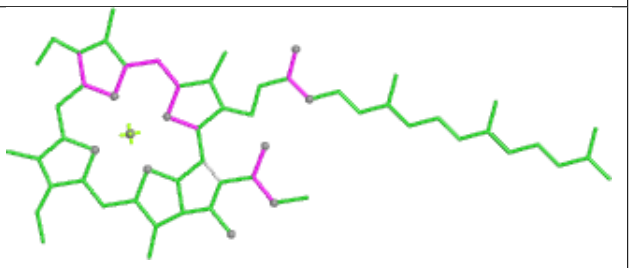

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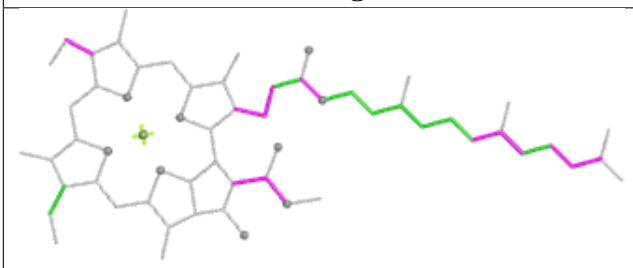

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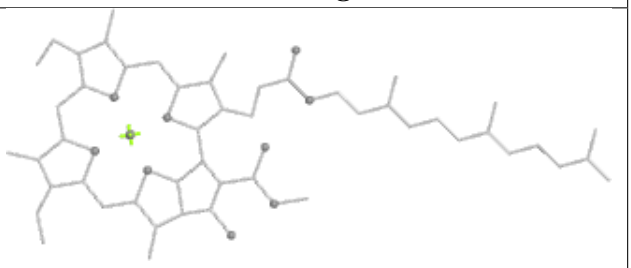
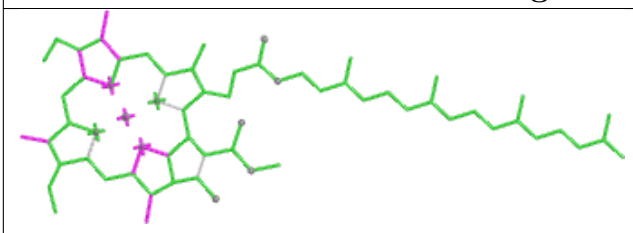


Rings

Ligand CLA I 102



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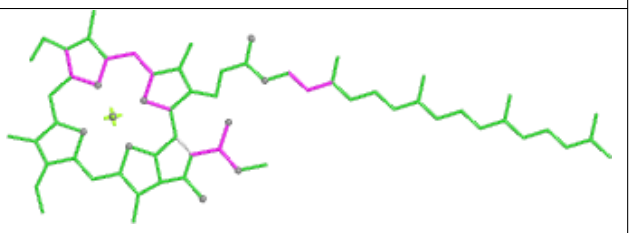

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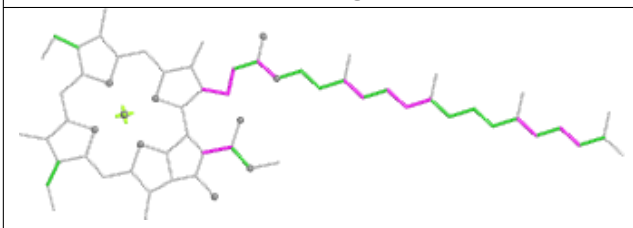

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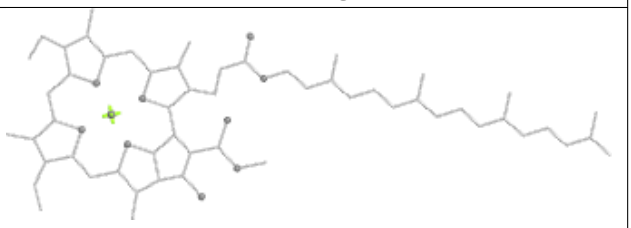
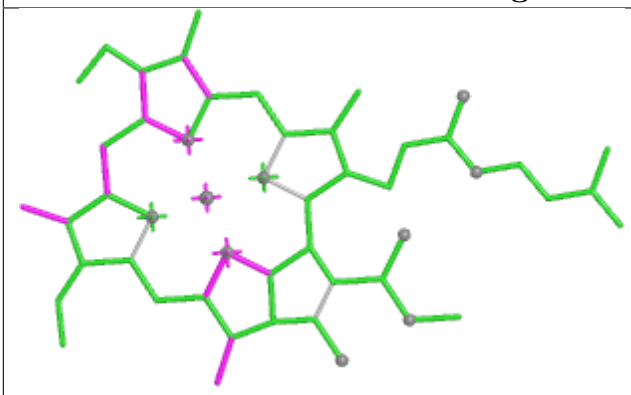
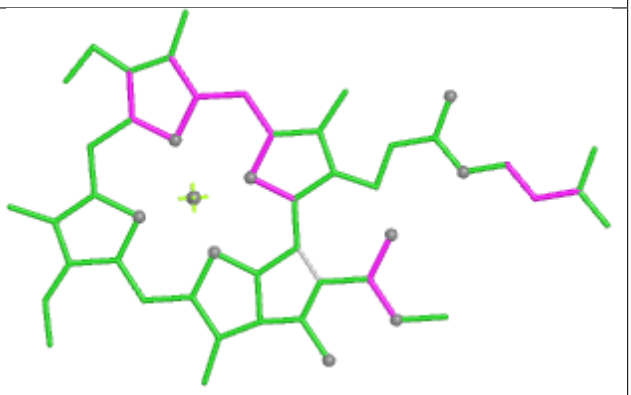
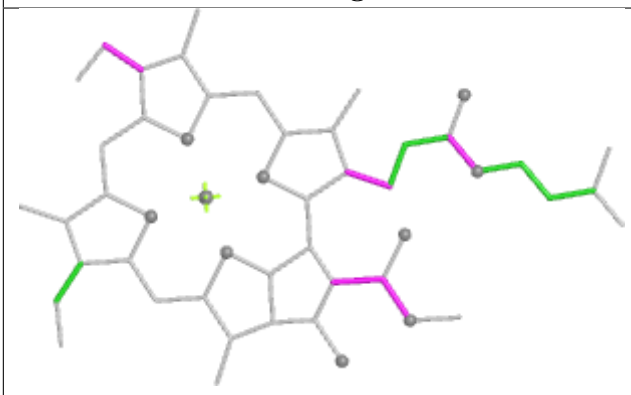
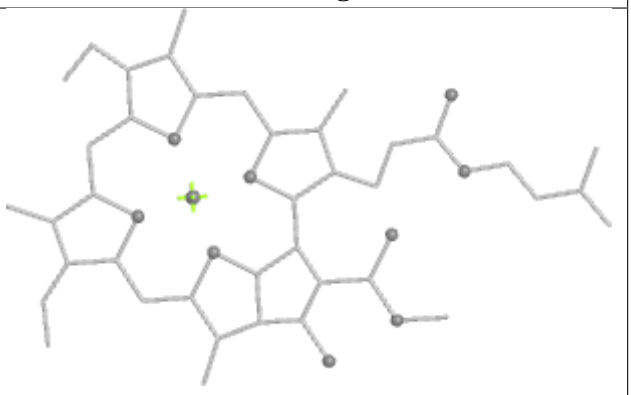


Rings

Ligand CLA BV 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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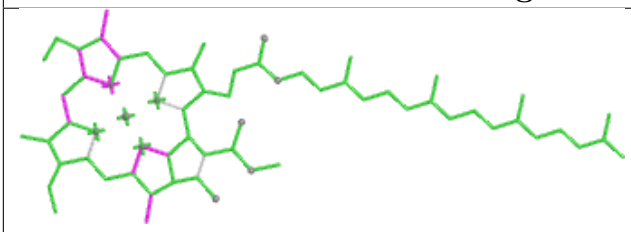
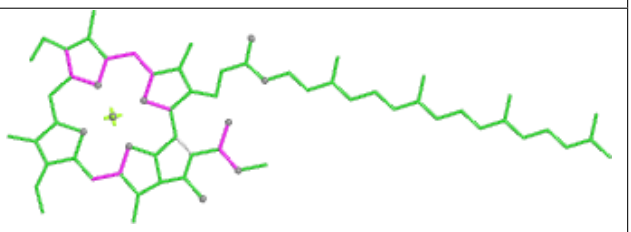
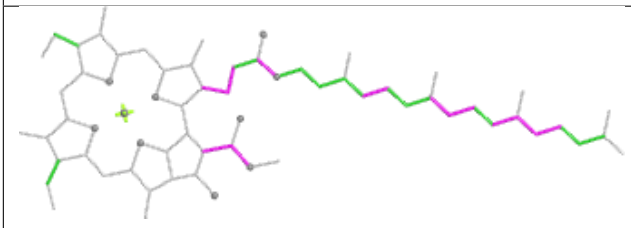
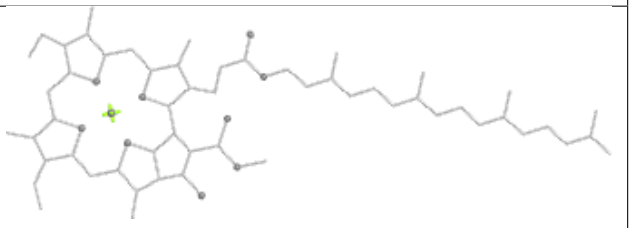
 Bond lengths	 Bond angles
 Torsions	 Rings

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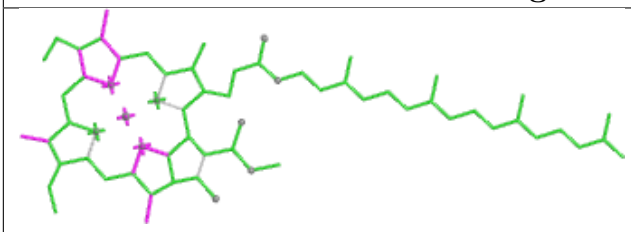
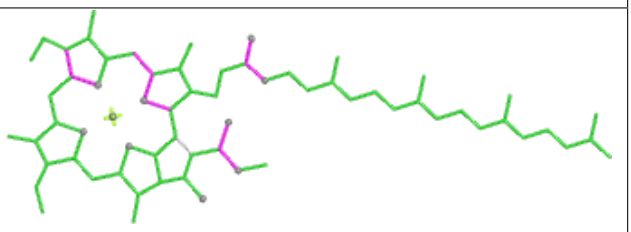
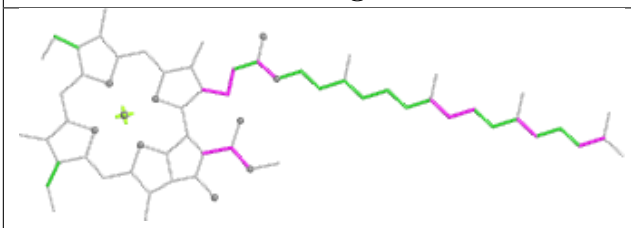
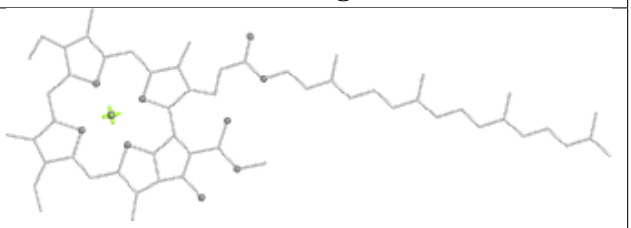
 Bond lengths	 Bond angles
 Torsions	 Rings

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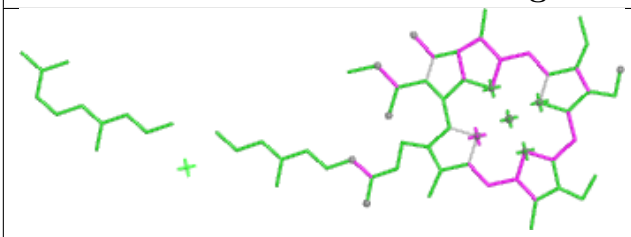
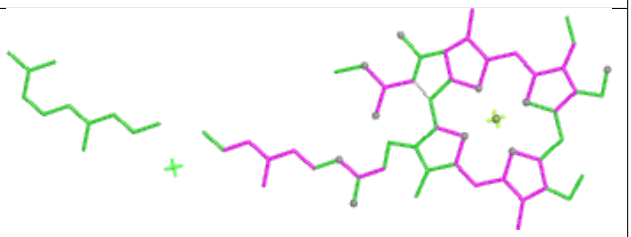
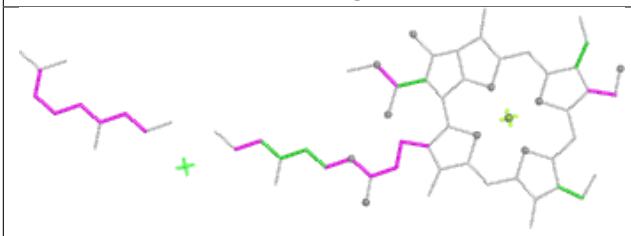
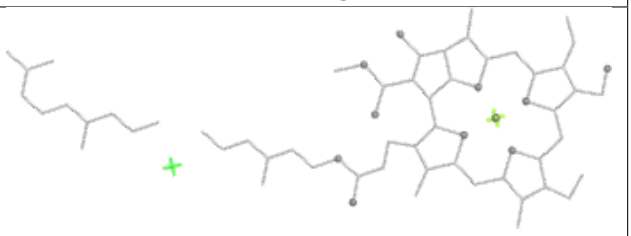
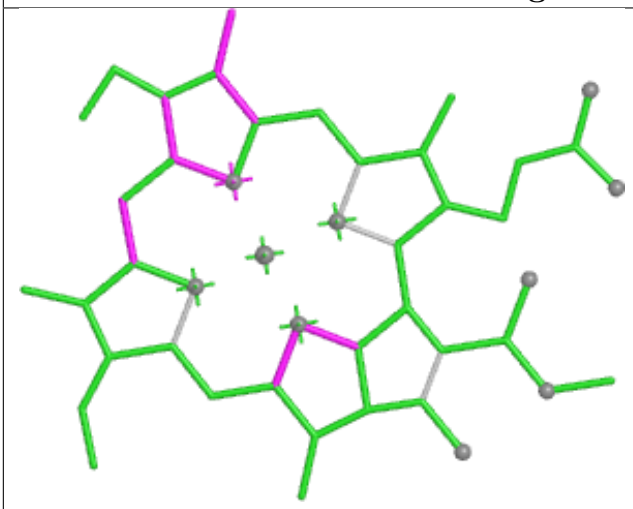
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 614



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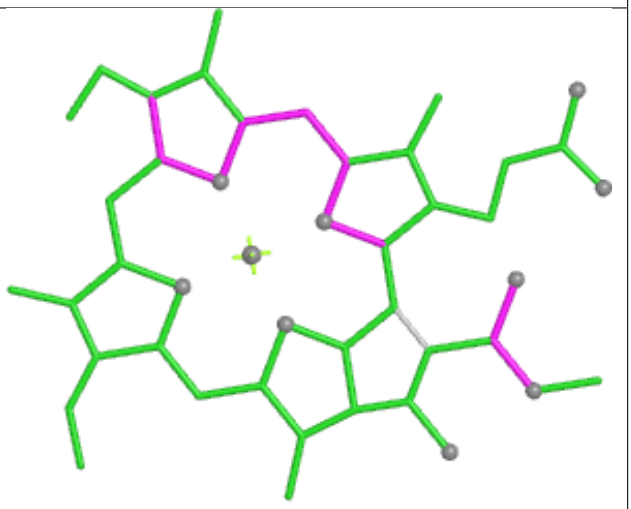

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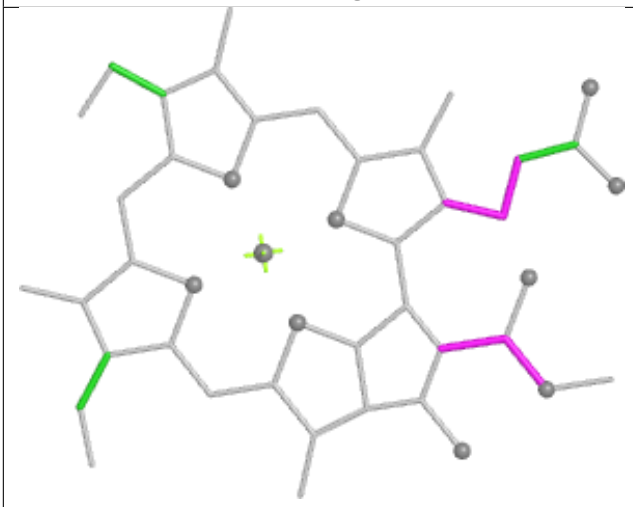
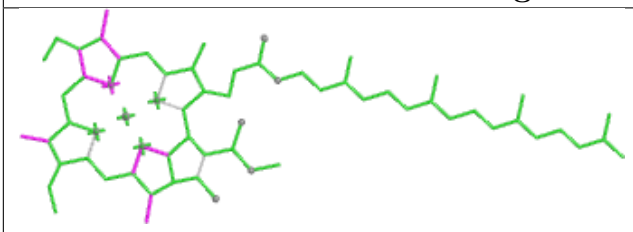


Torsions

Rings

Ligand CLA Au 613



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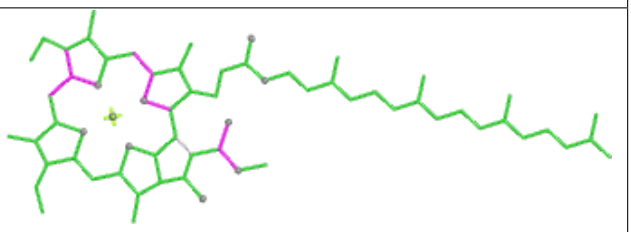

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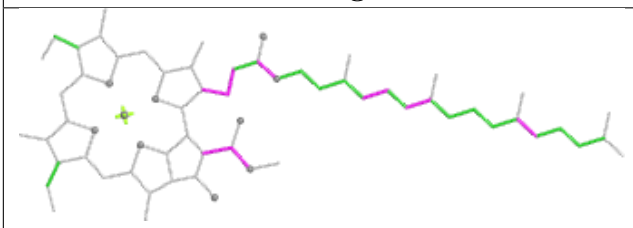

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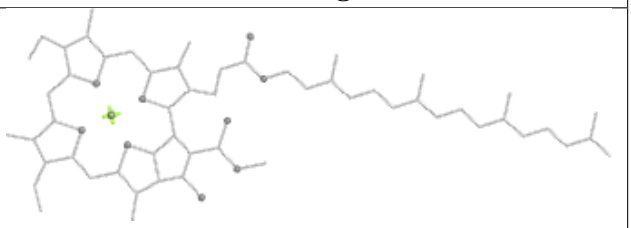
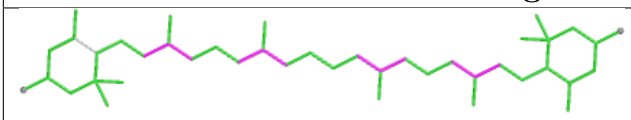


Rings

Ligand LUT G 616



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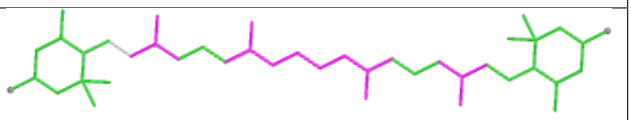

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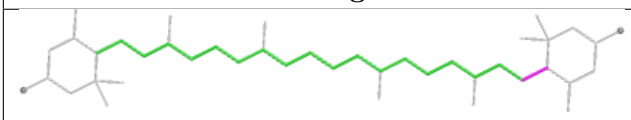

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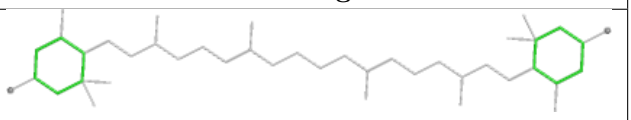
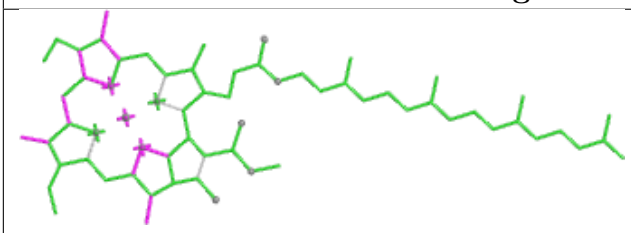


Rings

Ligand CLA BE 613



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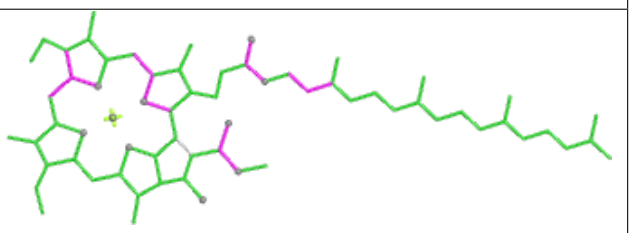

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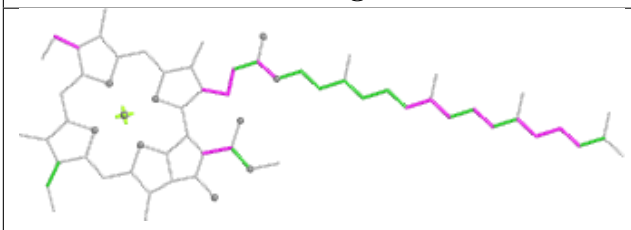

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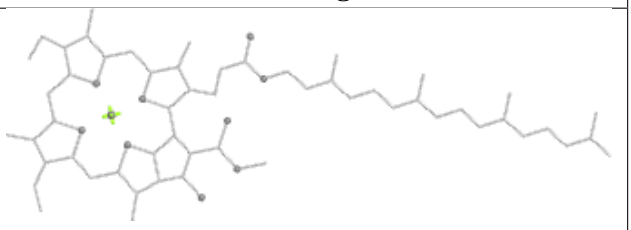
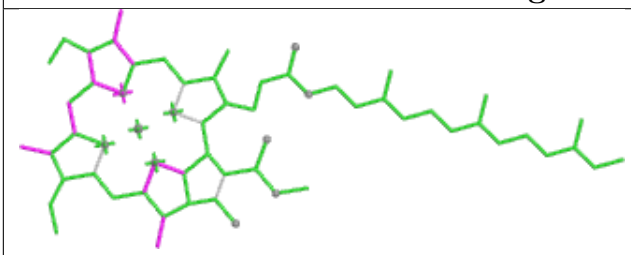


Rings

Ligand CLA 5 602



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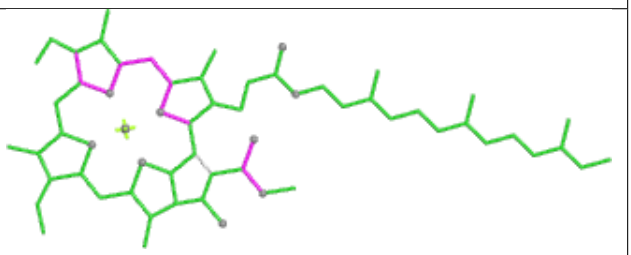

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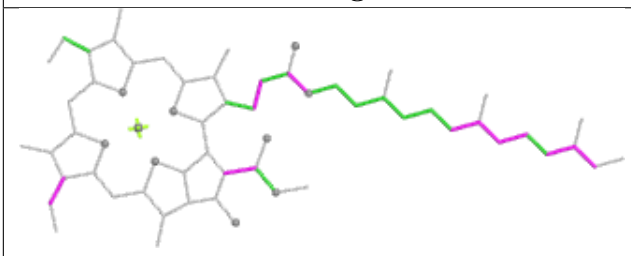

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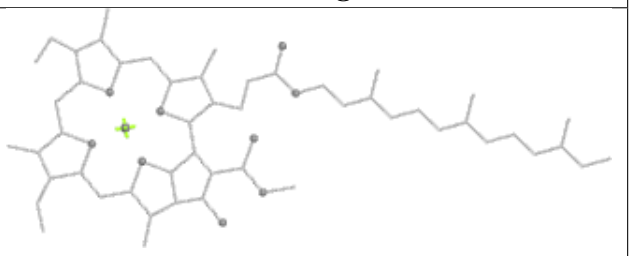
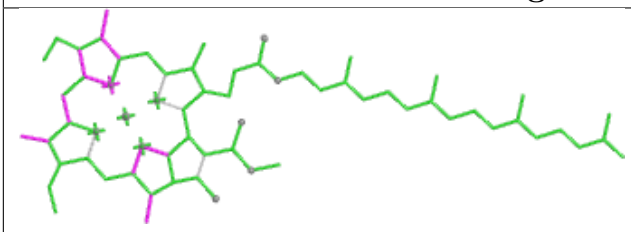


Rings

Ligand CLA v 605



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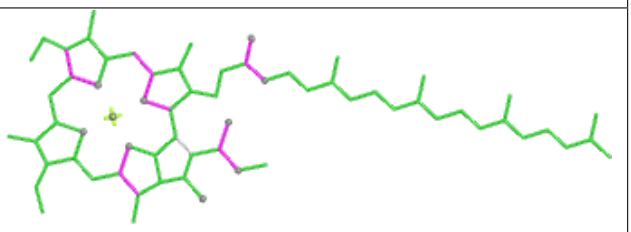

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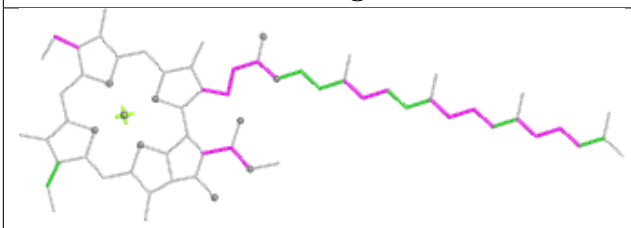

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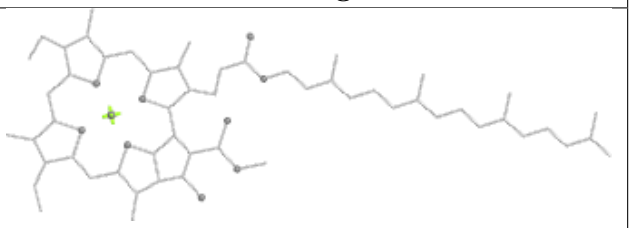
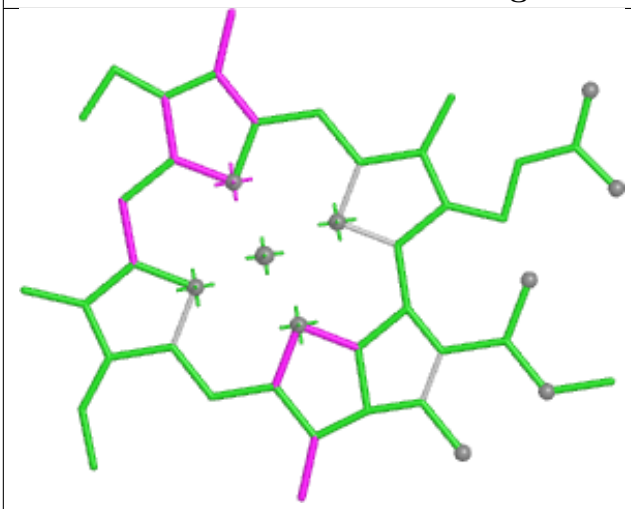
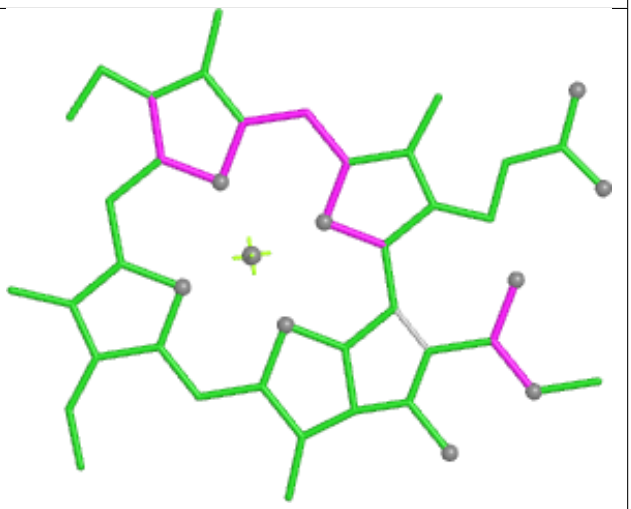


Rings

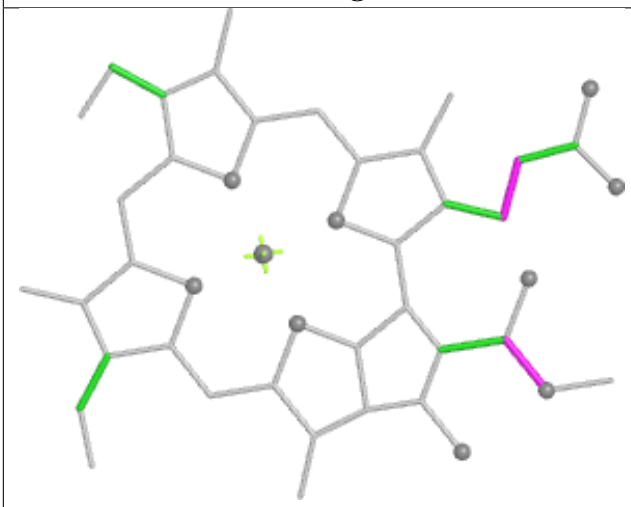
Ligand CLA AA 315



Bond lengths



Bond angles



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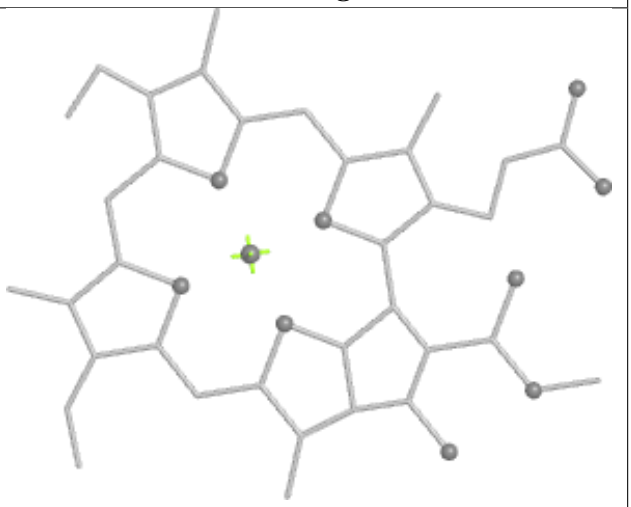
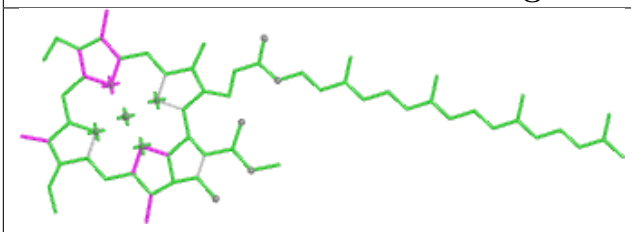
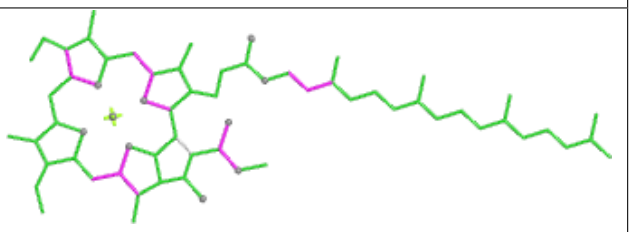
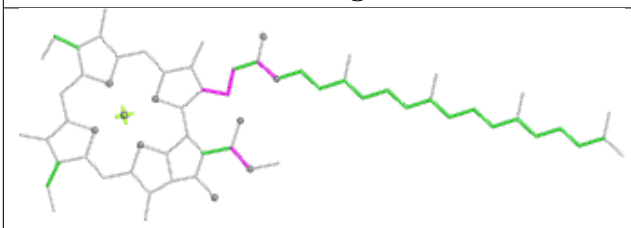
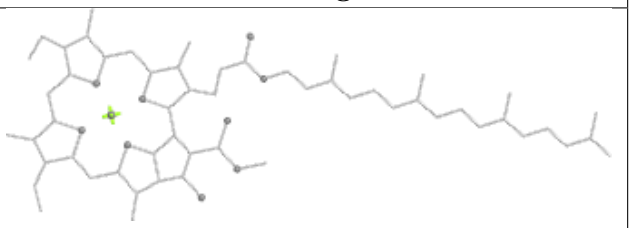


Rings

Ligand CLA R 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

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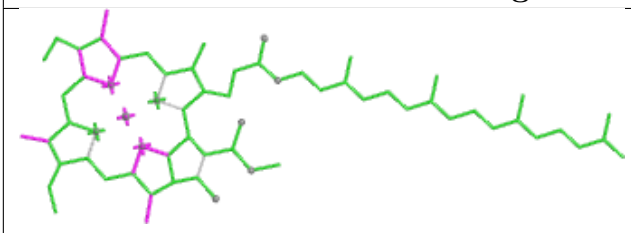
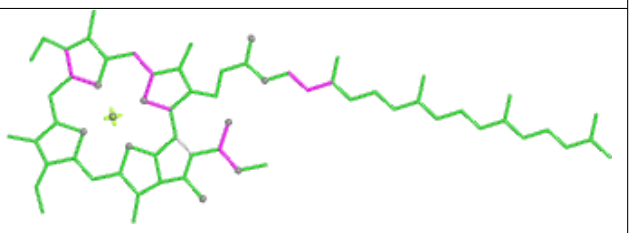
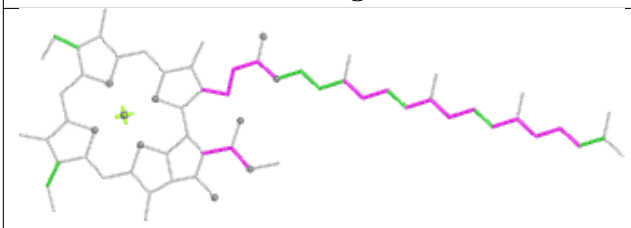
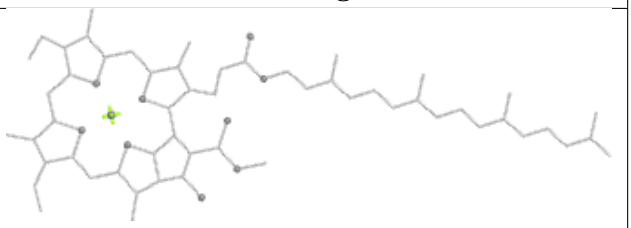
 Bond lengths	 Bond angles
 Torsions	 Rings

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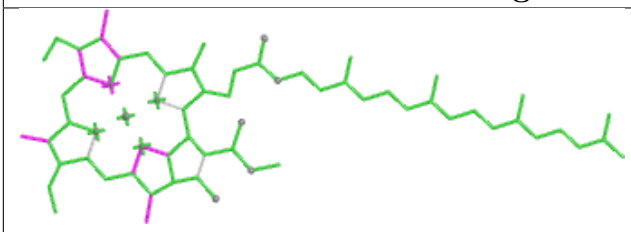
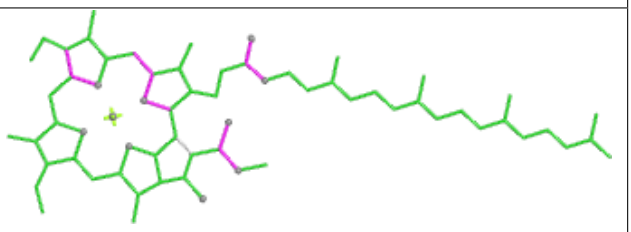
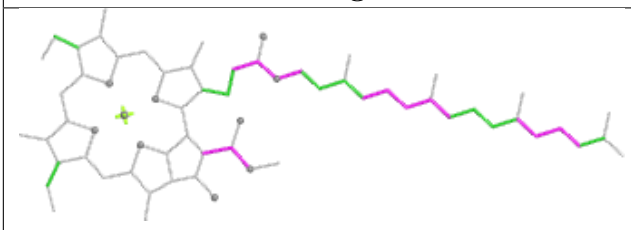
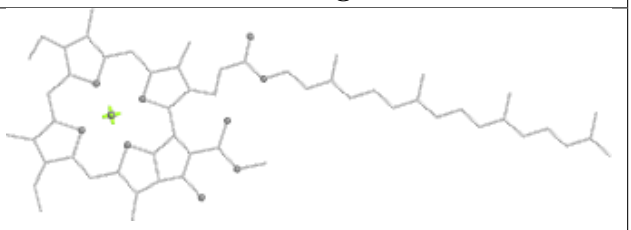
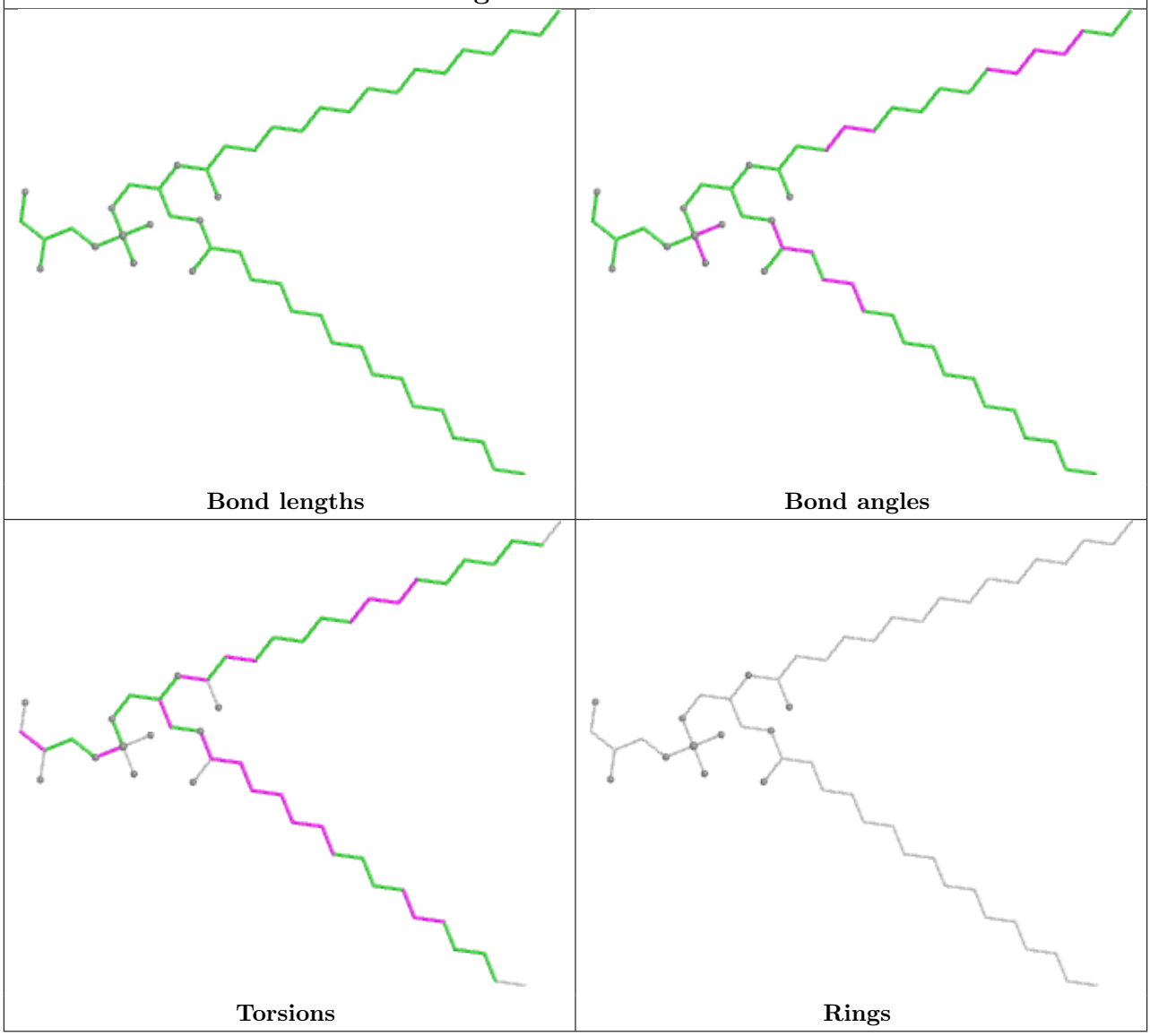
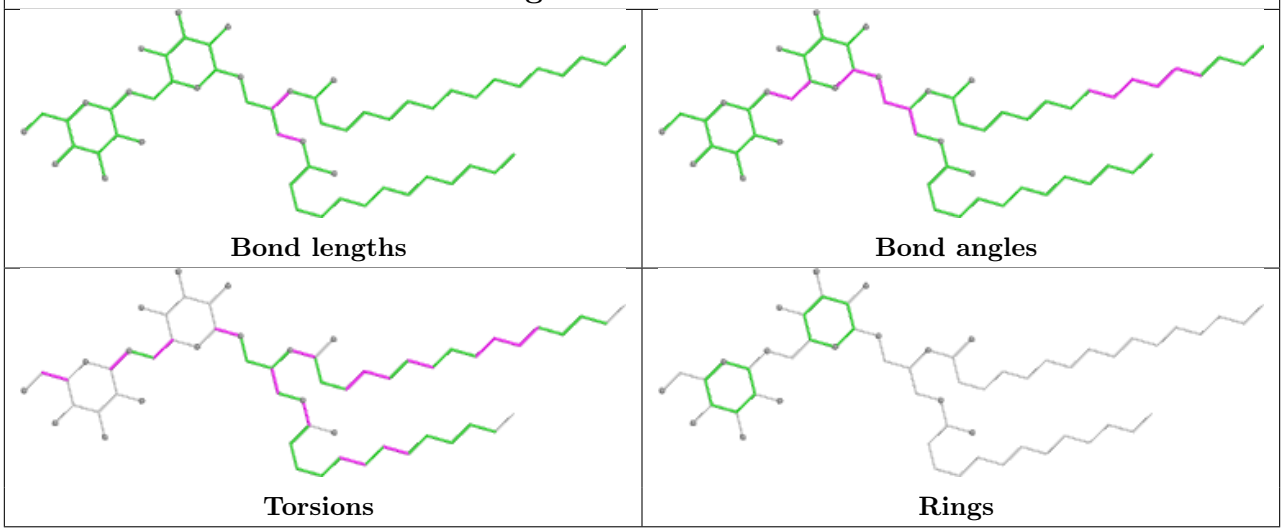
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG c 520



Ligand DGD a 401



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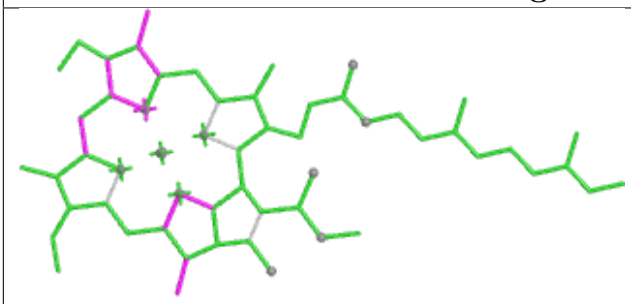
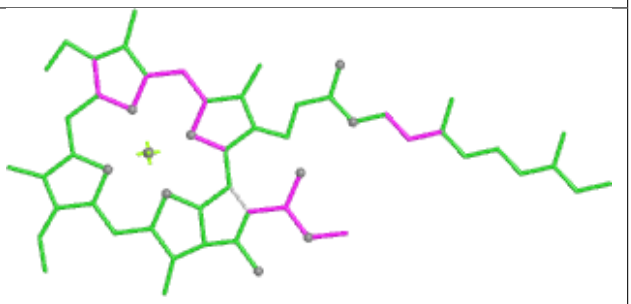
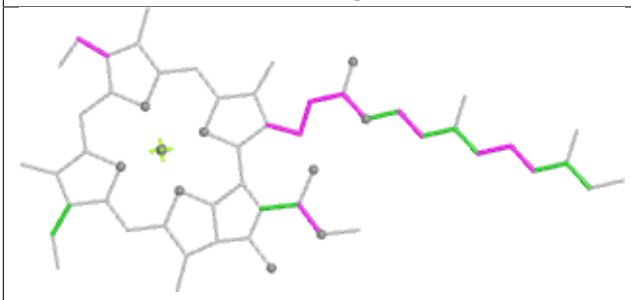
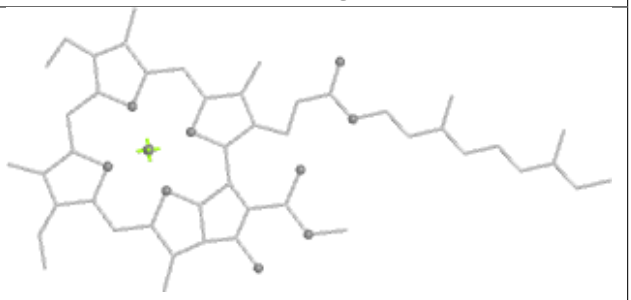
 Bond lengths	 Bond angles
 Torsions	 Rings

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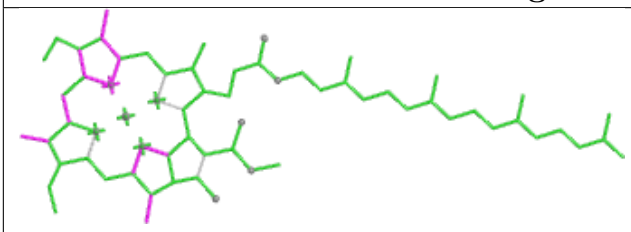
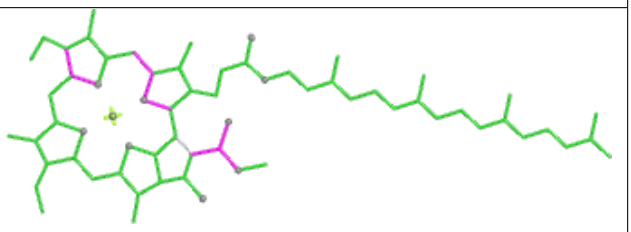
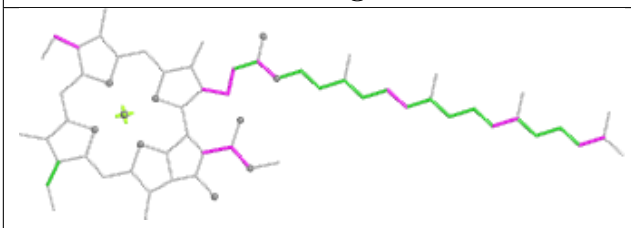
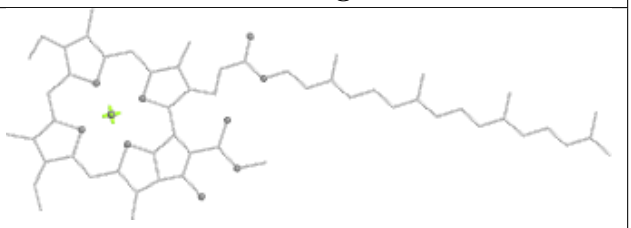
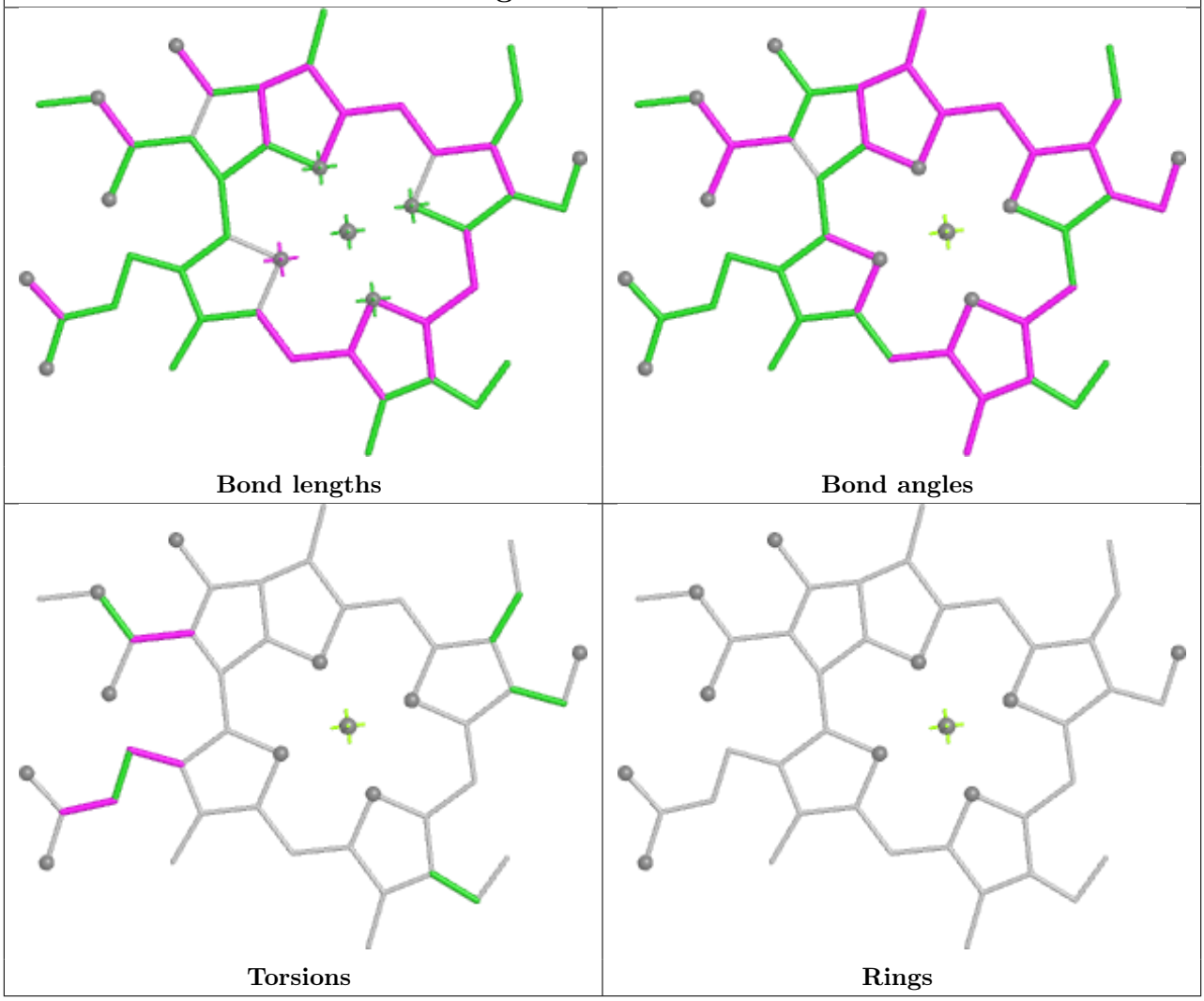
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 7 302



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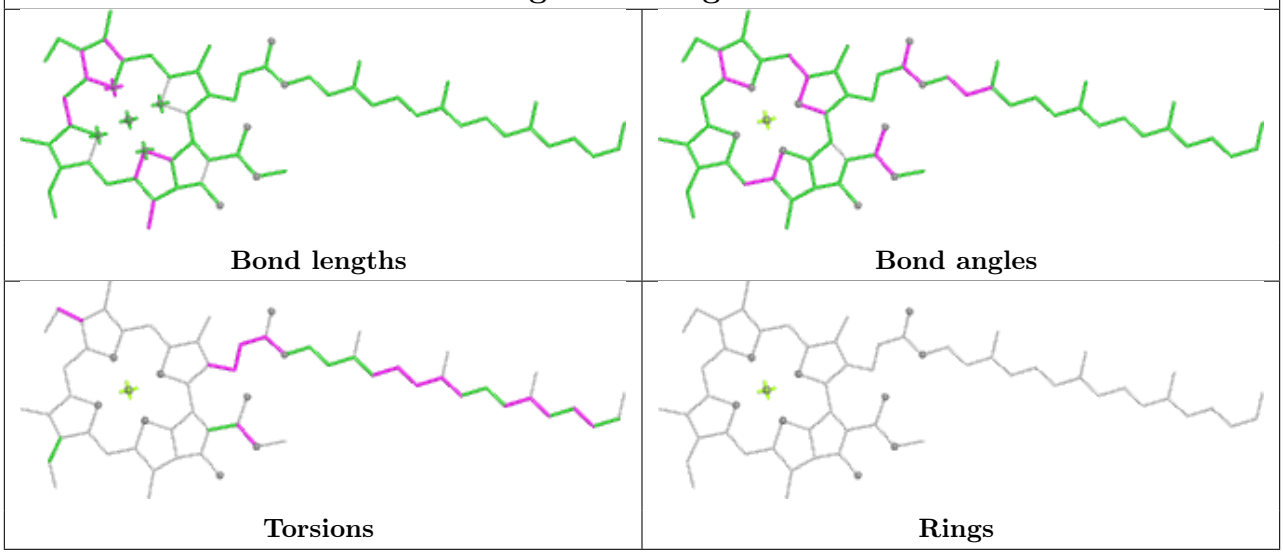

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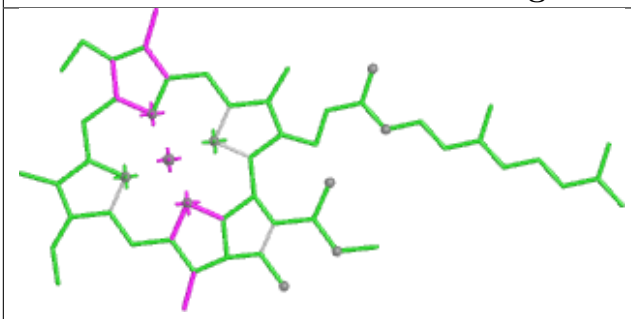
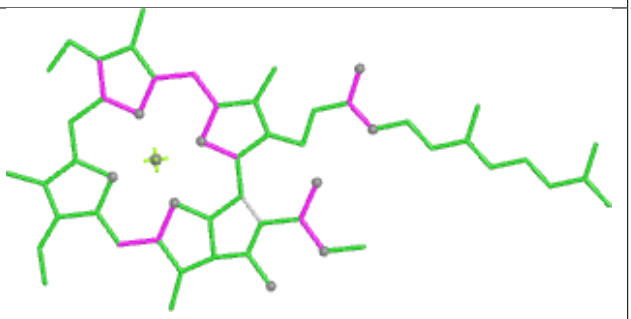
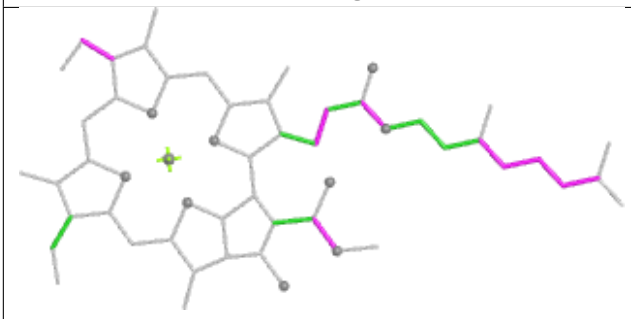


Bond lengths



Bond angles



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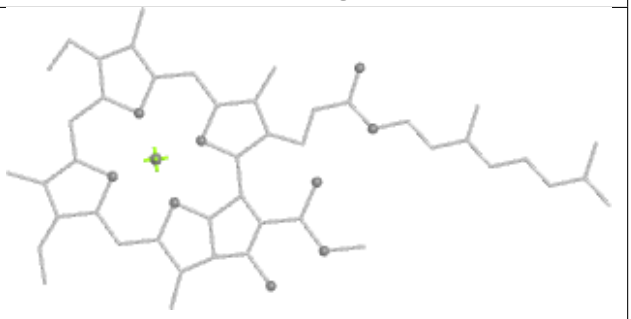

Rings

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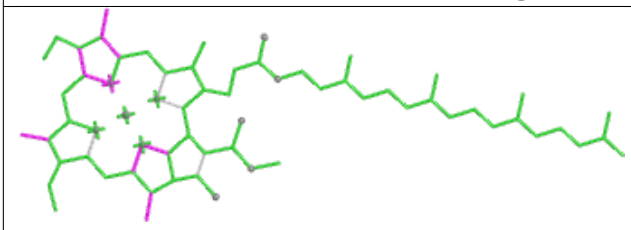

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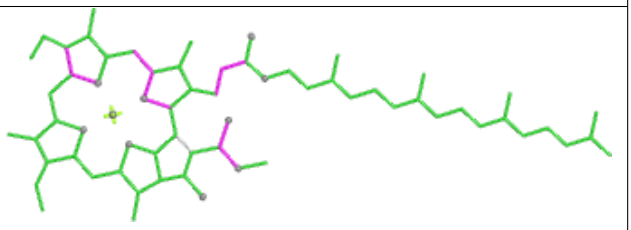
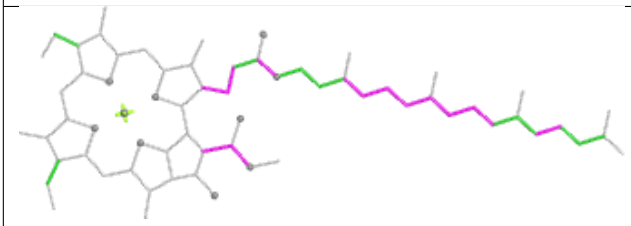


Bond angles



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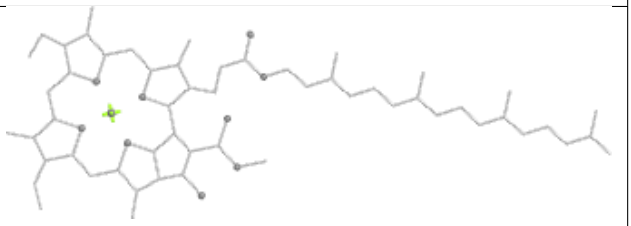
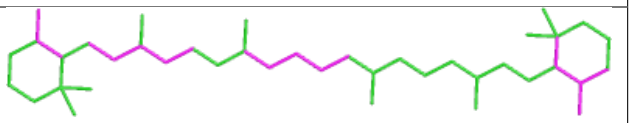


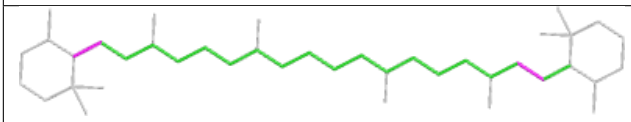
Rings

Ligand BCR b 618

Bond lengths



Bond angles



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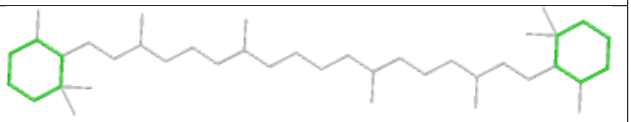

Rings

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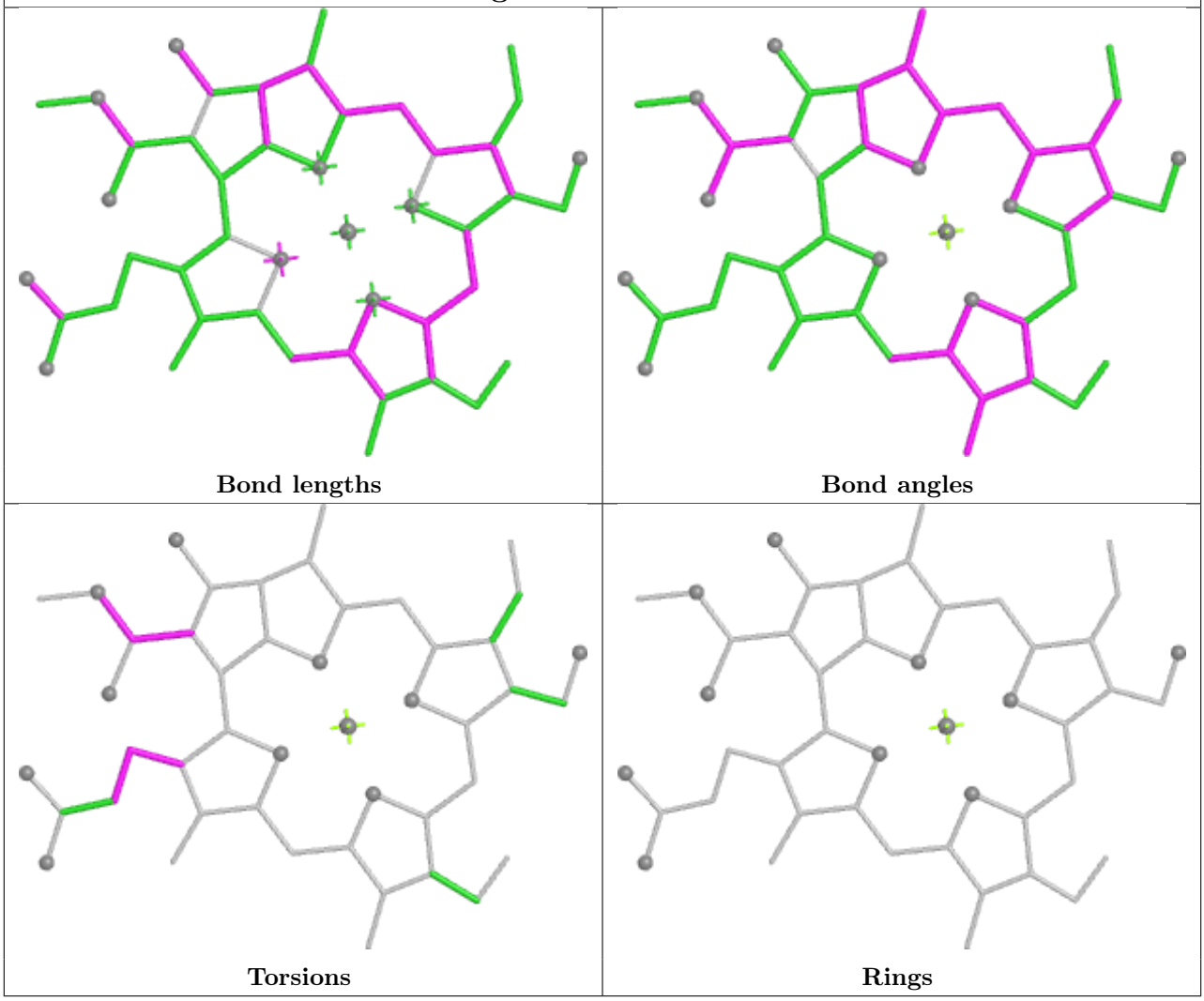
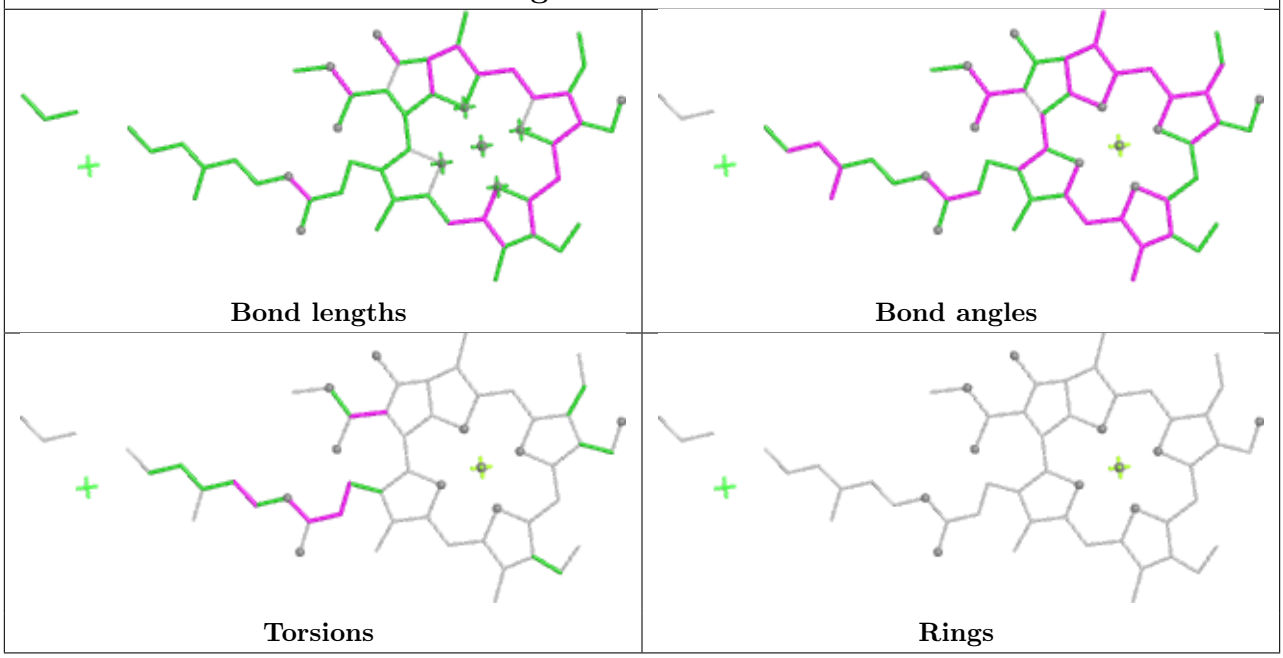
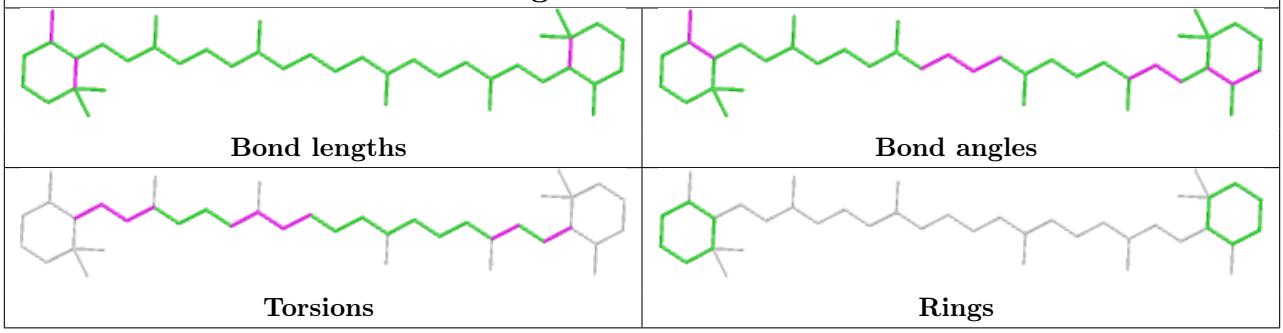


Ligand CHL s 606



Ligand BCR f 101



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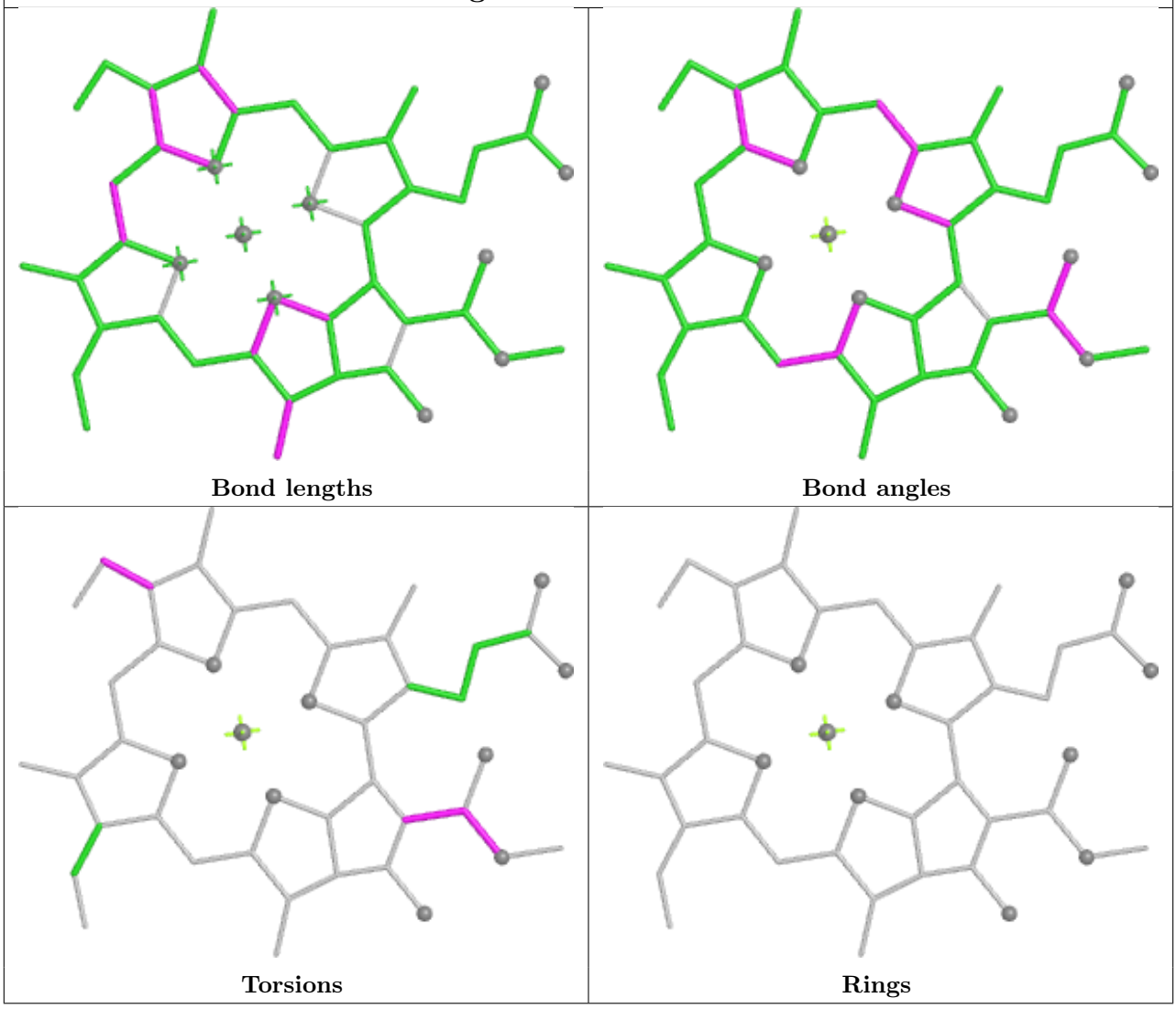

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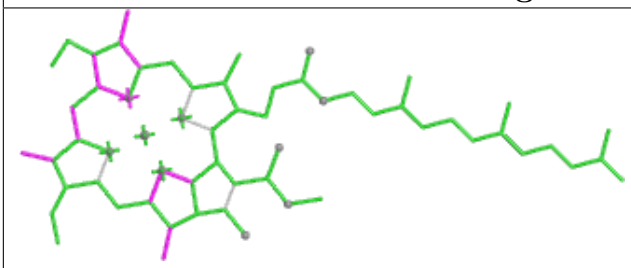
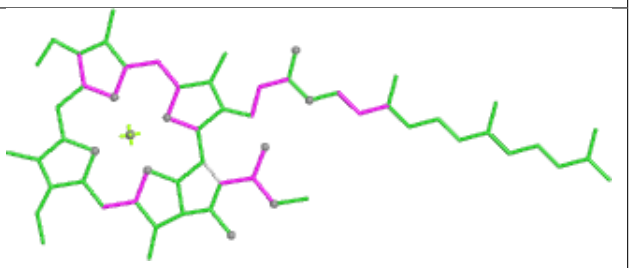
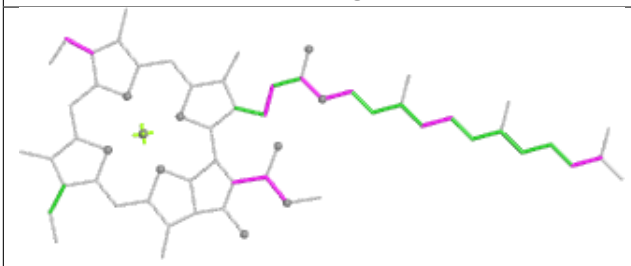
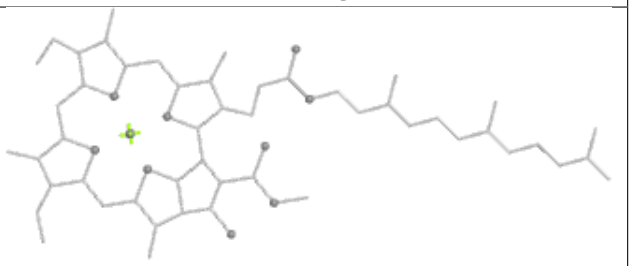
 Bond lengths	 Bond angles
 Torsions	 Rings

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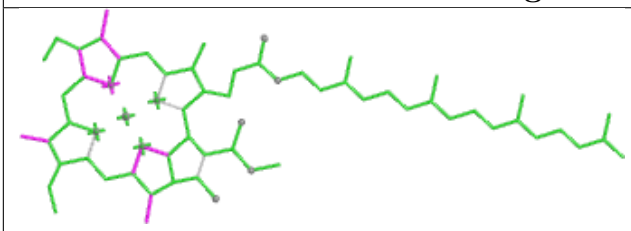
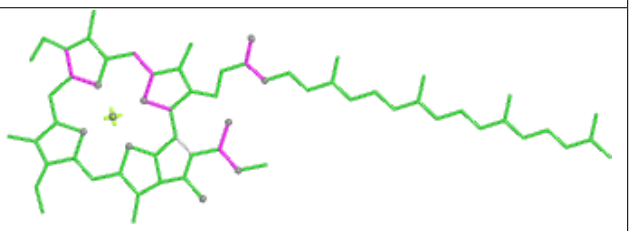
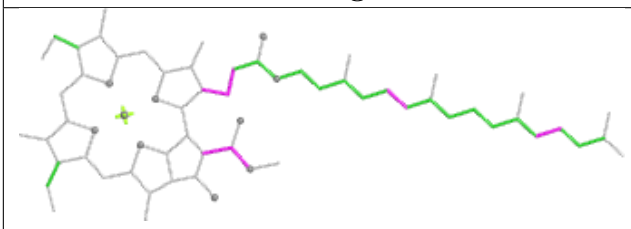
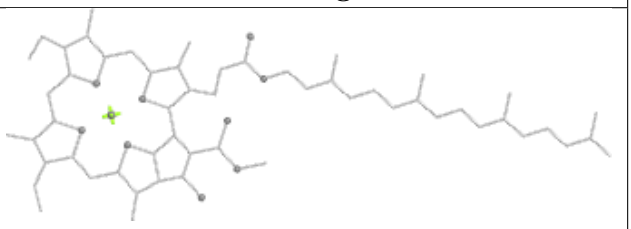
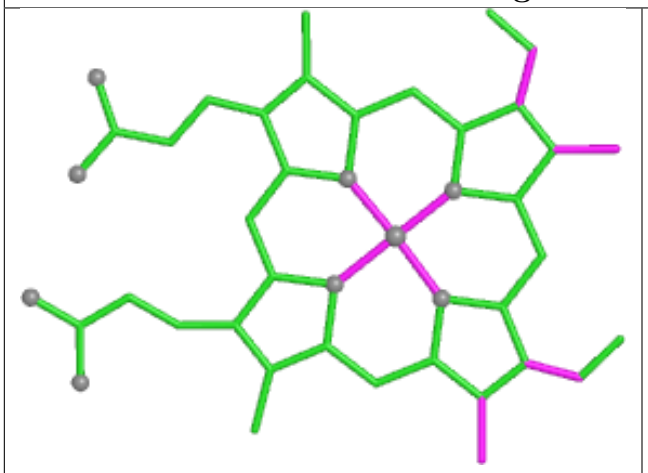
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM BI 102



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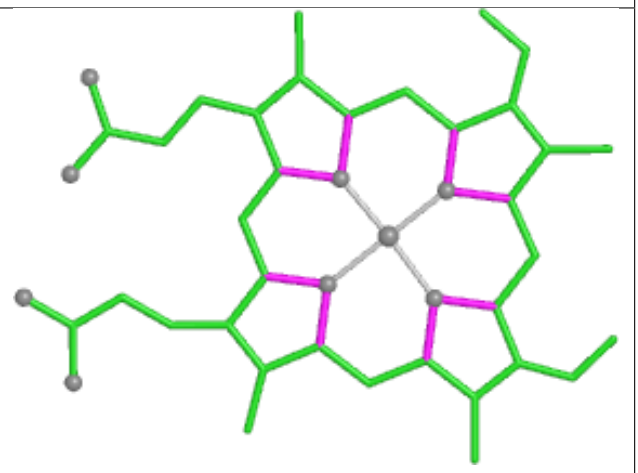
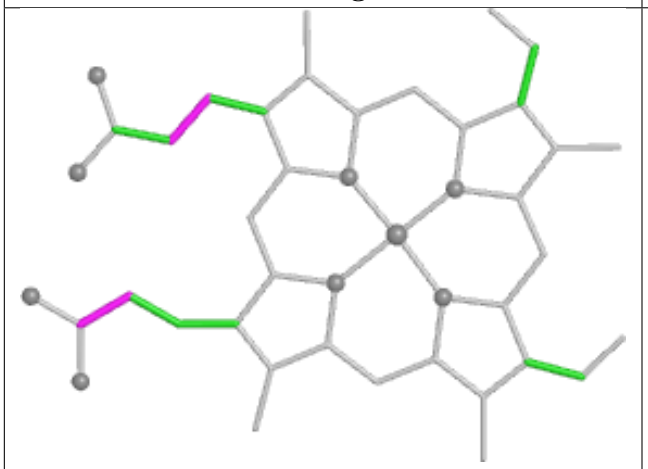
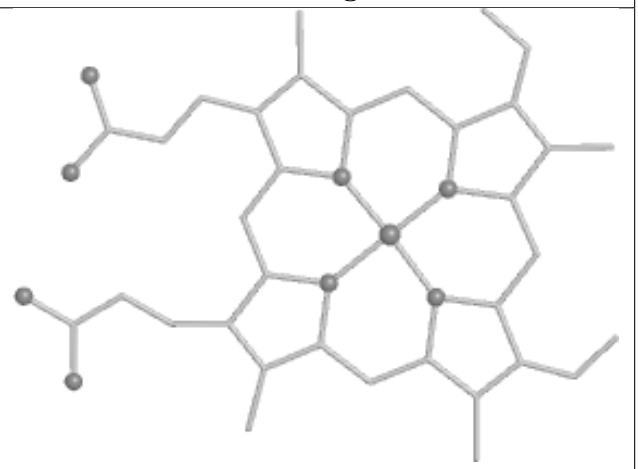


Bond angles

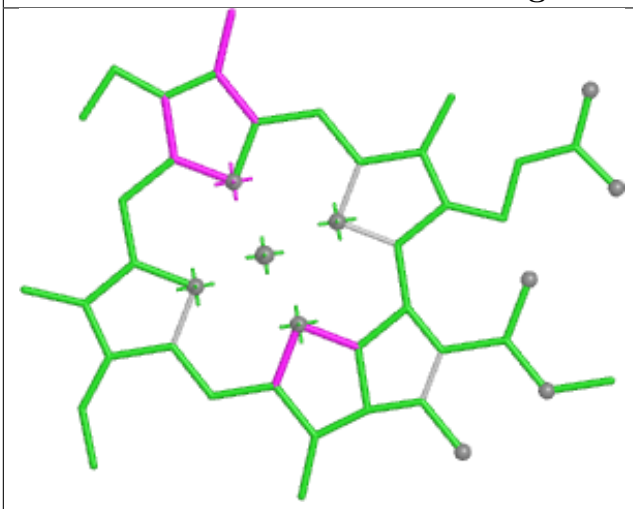


Torsions



Rings

Ligand CLA 9 614



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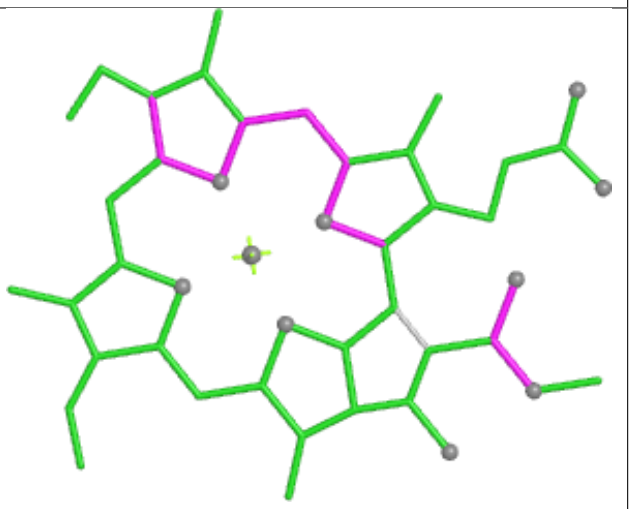
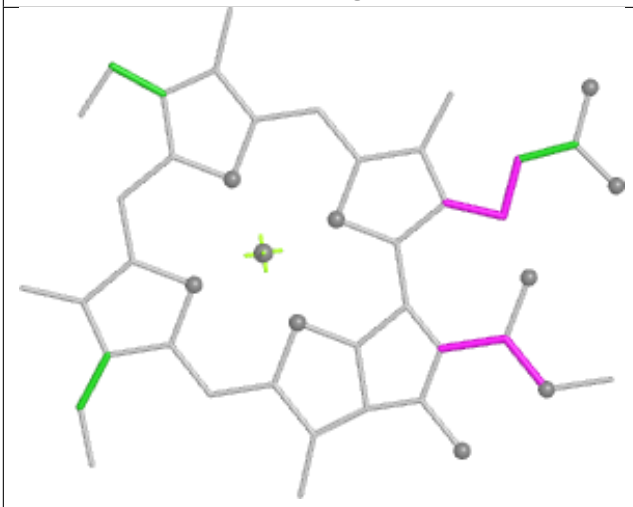


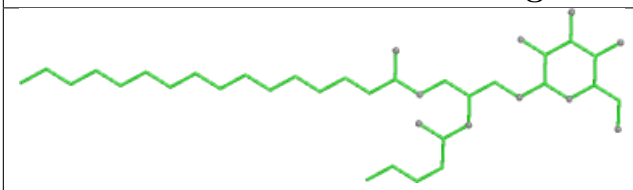
Bond angles



Torsions

Rings

Ligand LMG I 101



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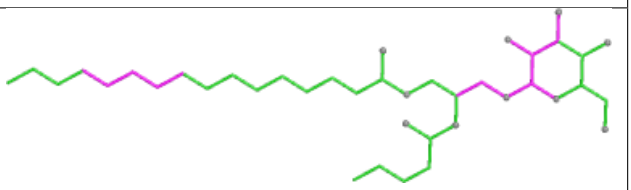

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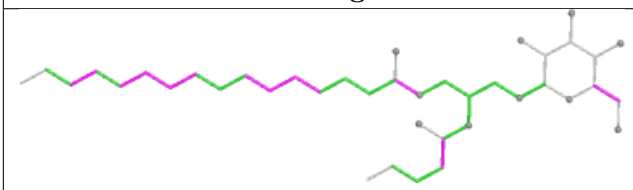
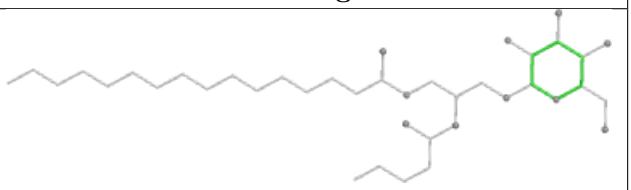
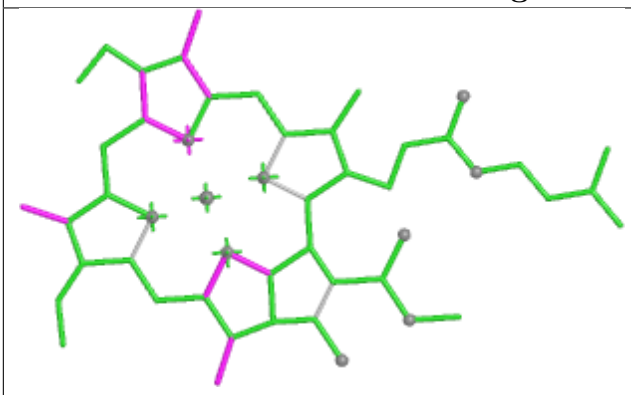
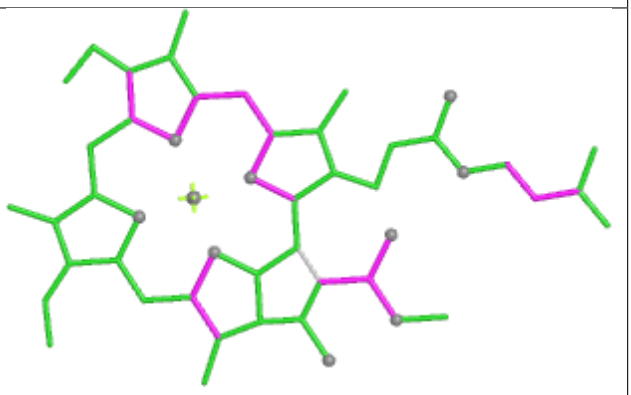
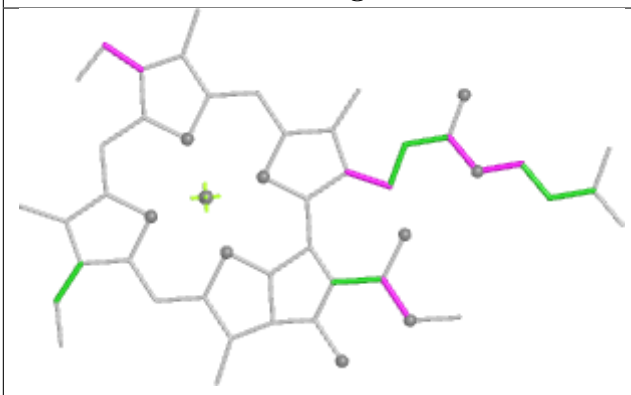
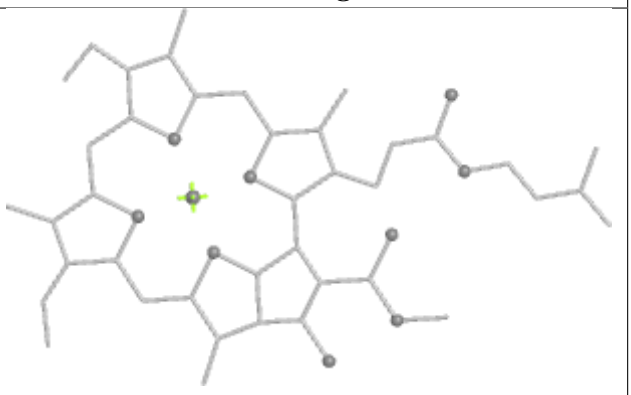


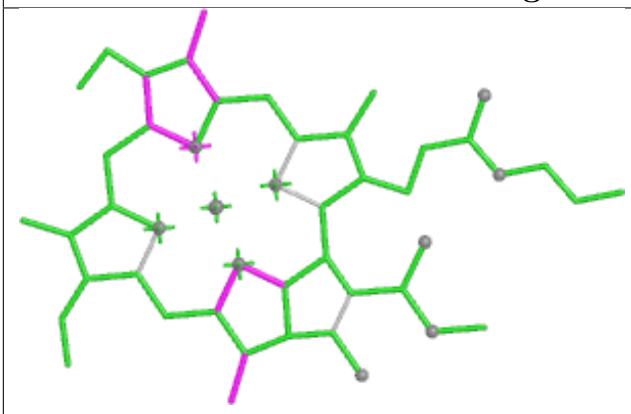
Torsions



Rings

Ligand CLA BD 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 614



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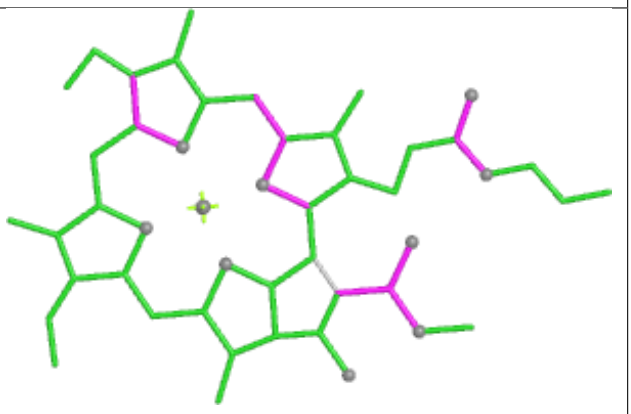

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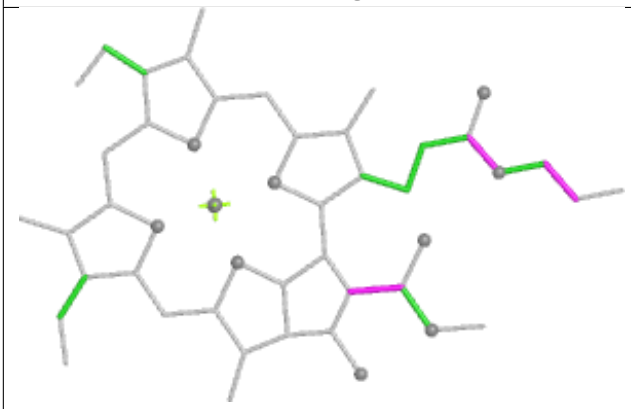

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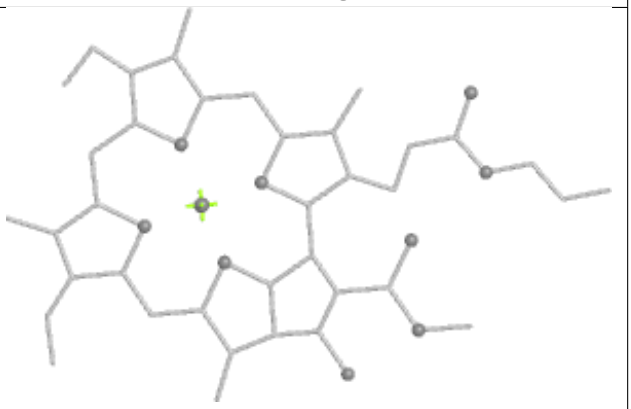
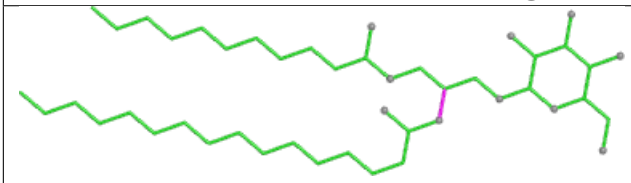


Rings

Ligand LMG d 405



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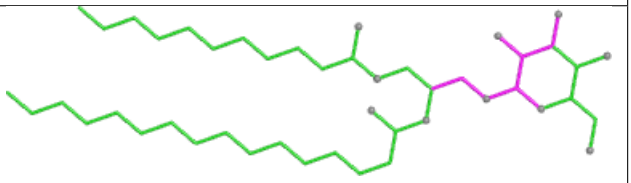
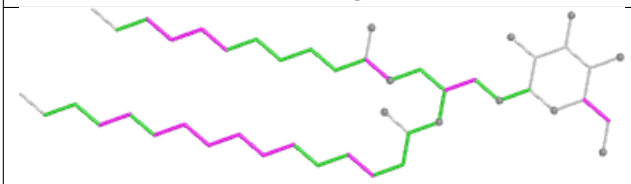


Bond angles



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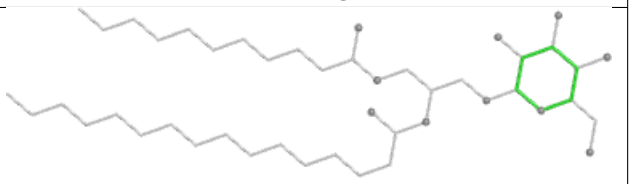
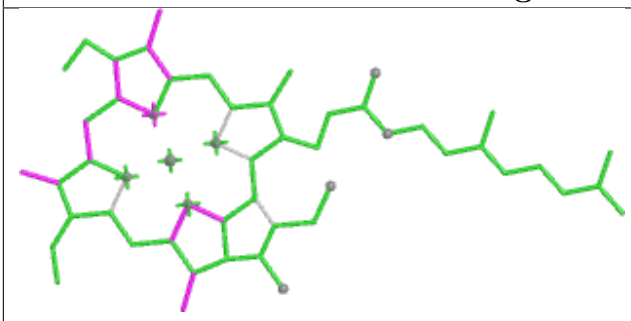


Rings

Ligand CLA A6 609



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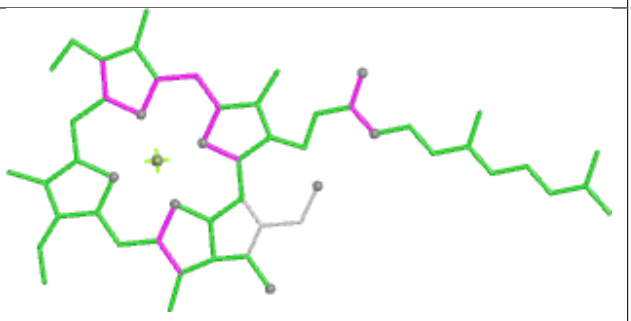

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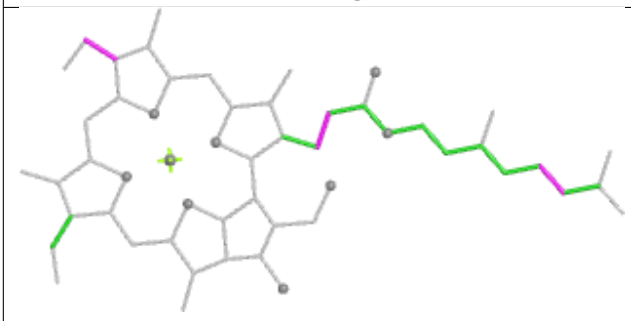

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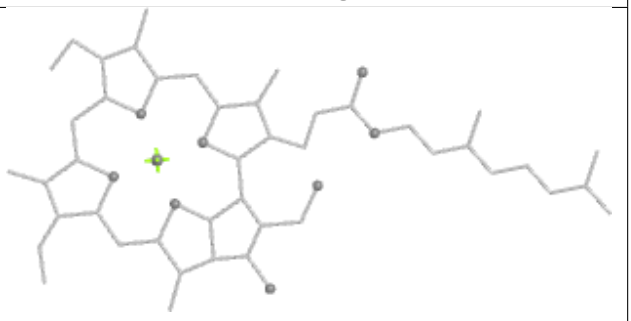
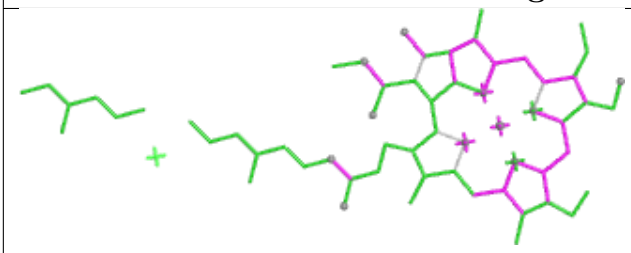


Rings

Ligand CHL 9 609



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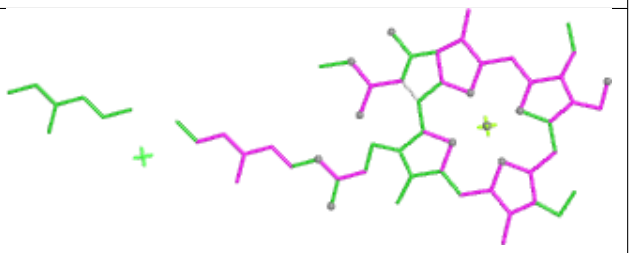
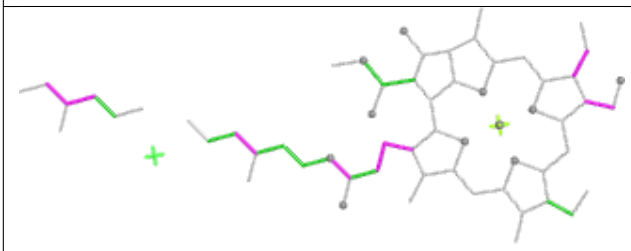


Bond angles



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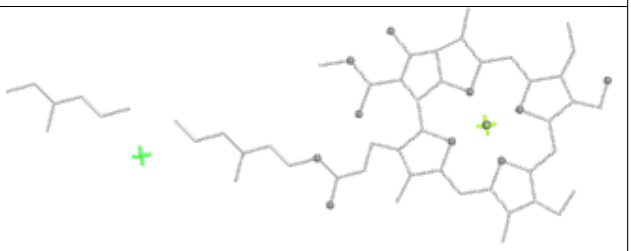
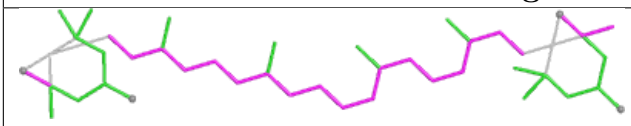


Rings

Ligand XAT N 619



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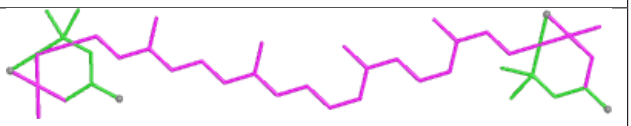
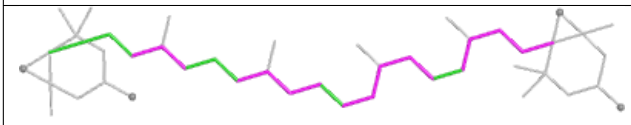


Bond angles



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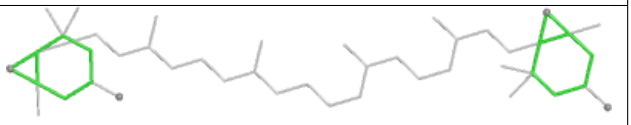
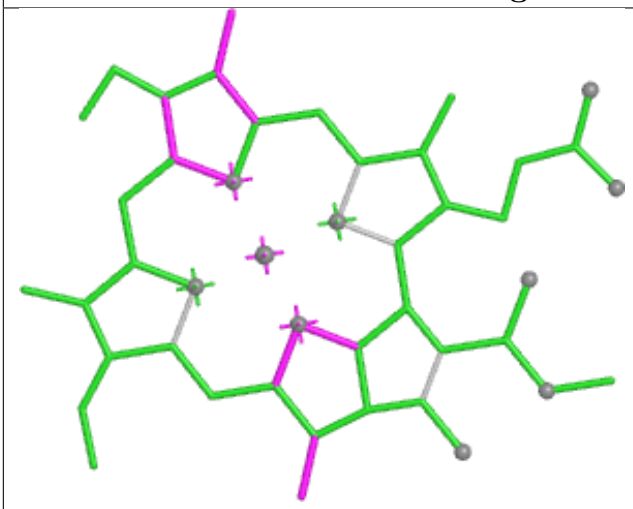


Rings

Ligand CLA AA 314



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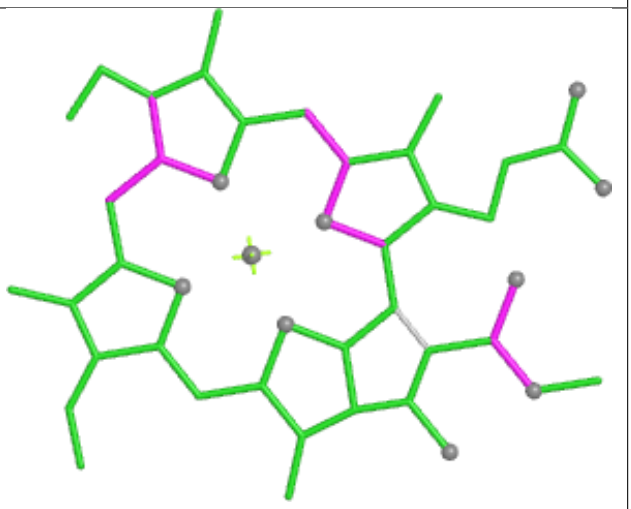

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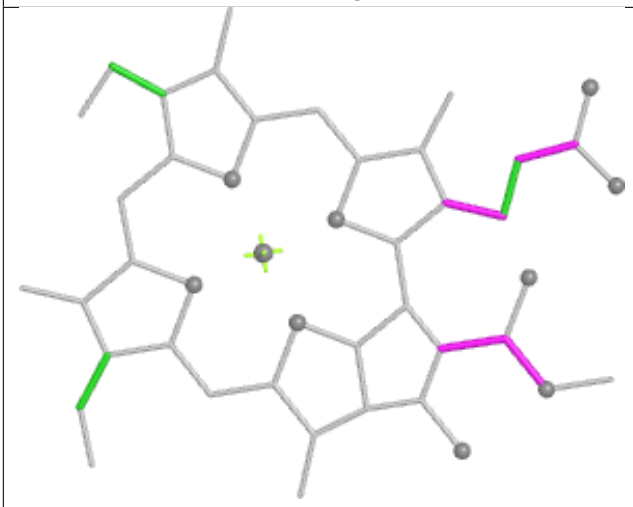
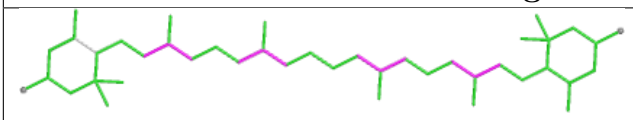


Torsions

Rings

Ligand LUT N 616



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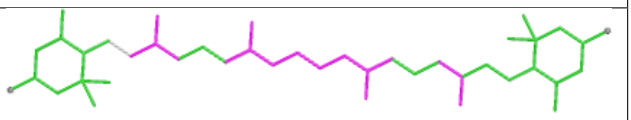

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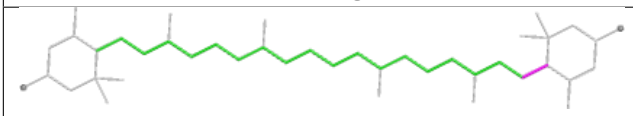

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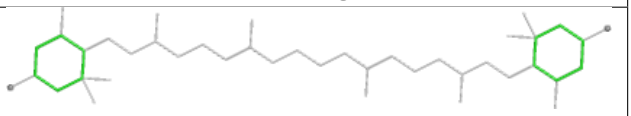
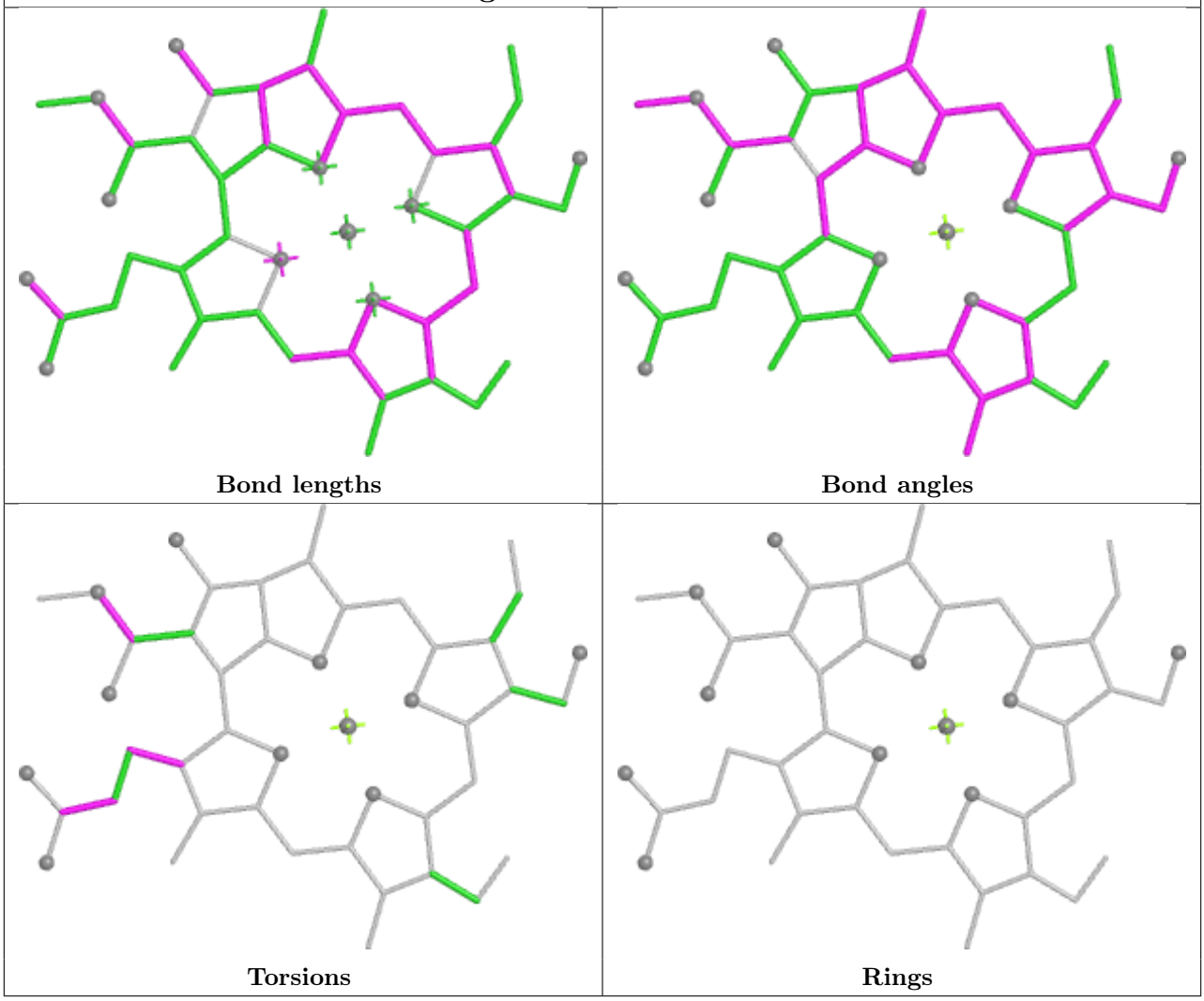
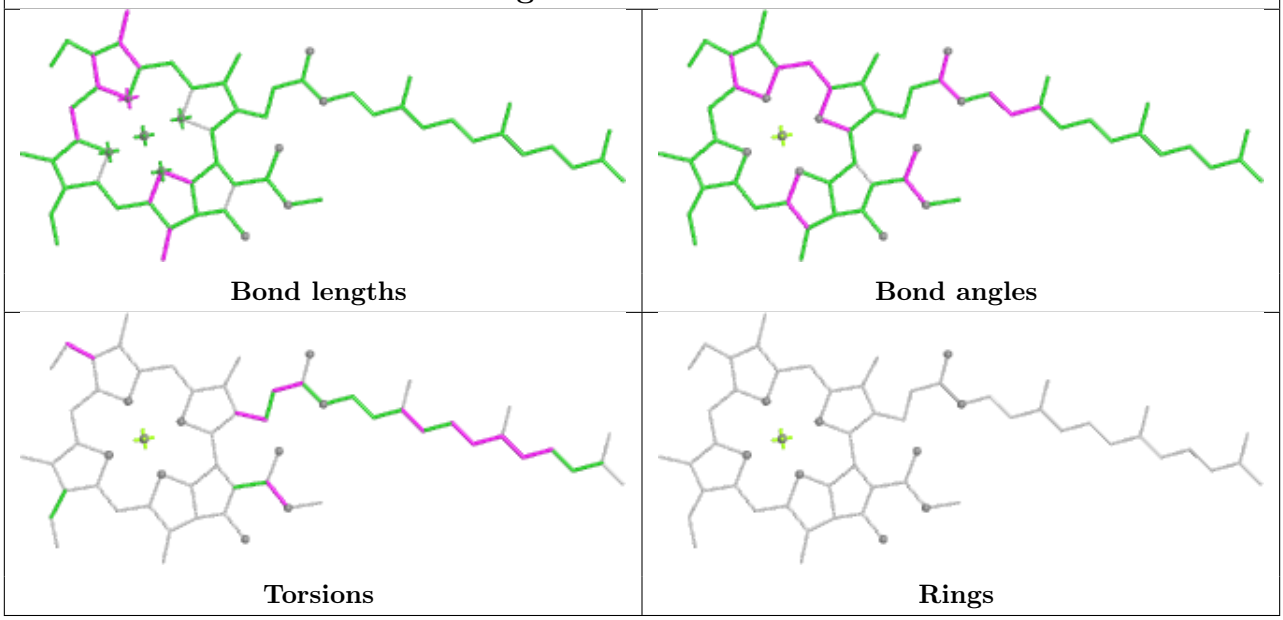


Rings

Ligand CHL AA 307



Ligand CLA Ba 312



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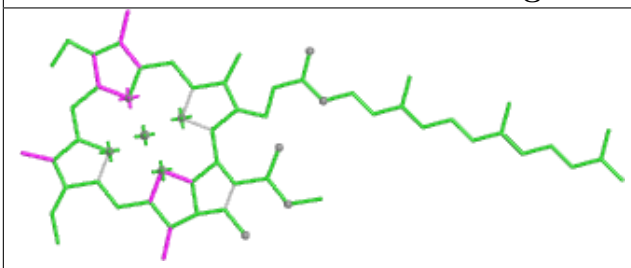
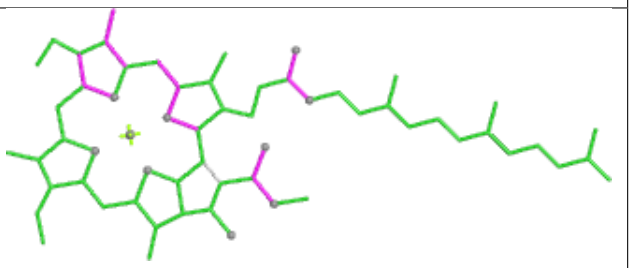
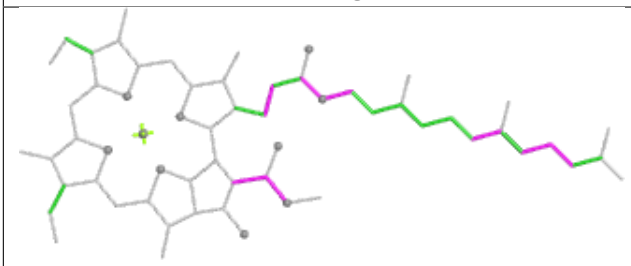
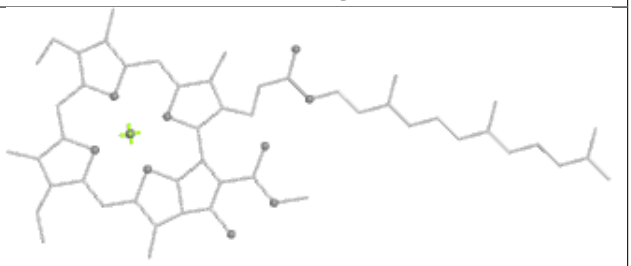
 Bond lengths	 Bond angles
 Torsions	 Rings

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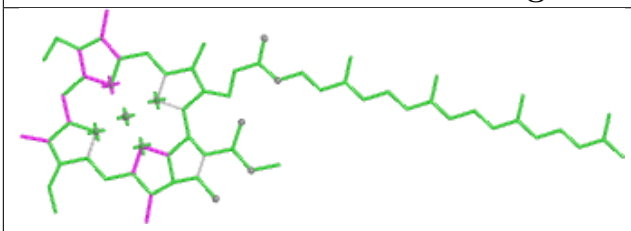
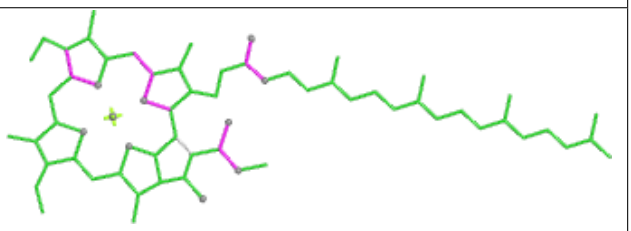
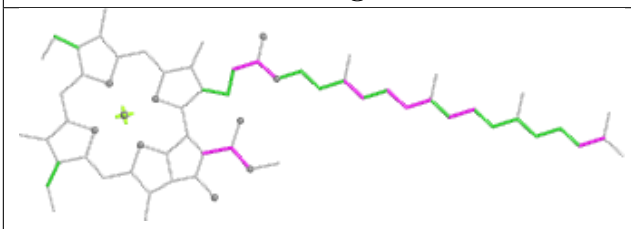
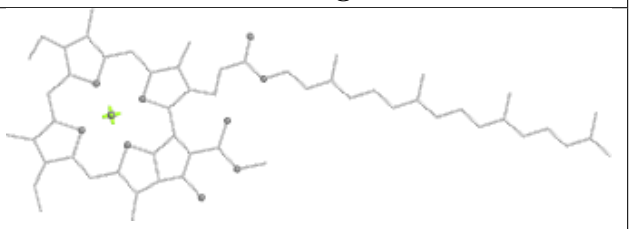
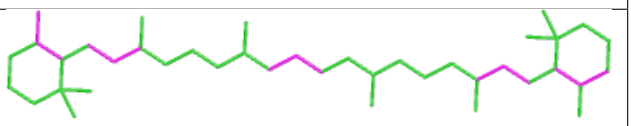
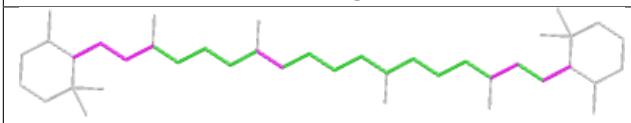
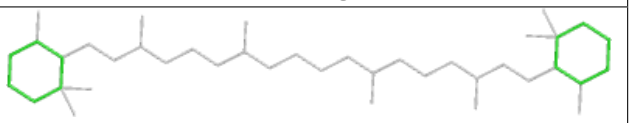
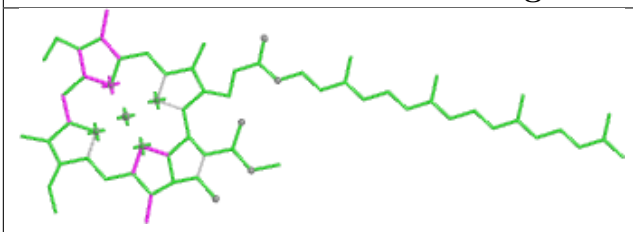
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 4 101	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 601



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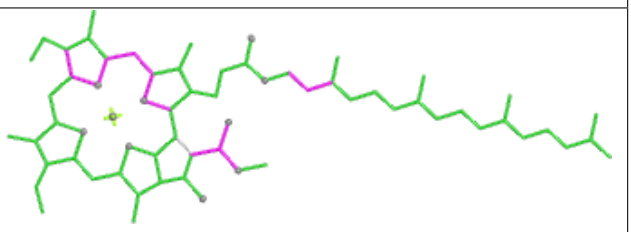
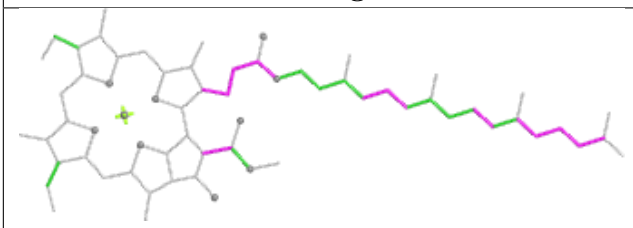


Bond angles



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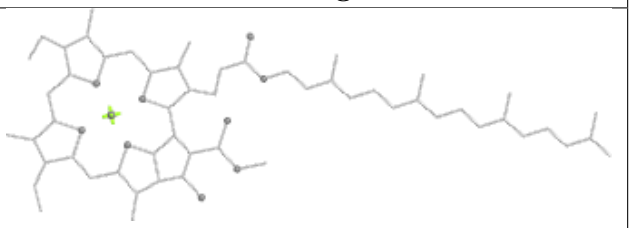
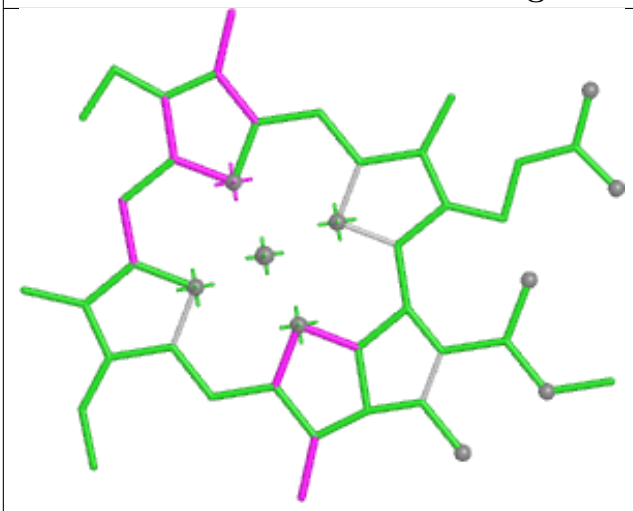


Rings

Ligand CLA S 608



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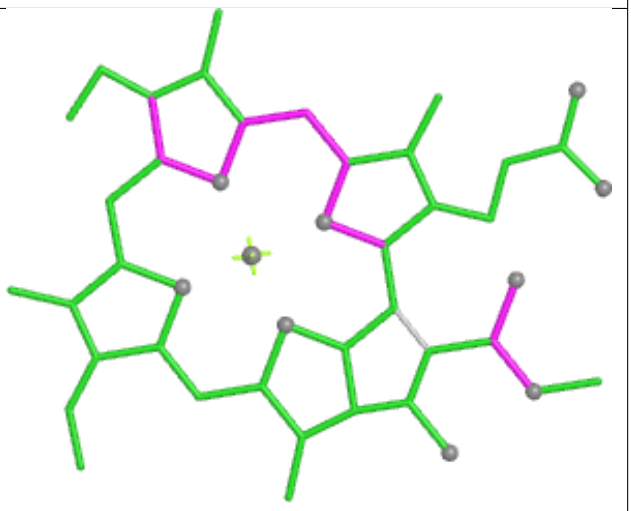

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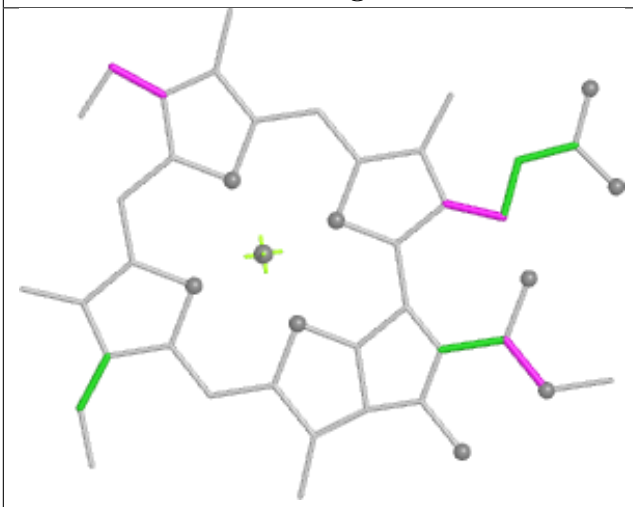

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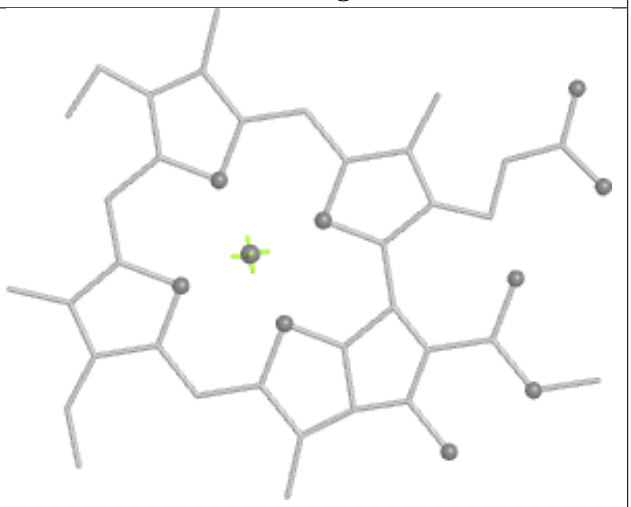
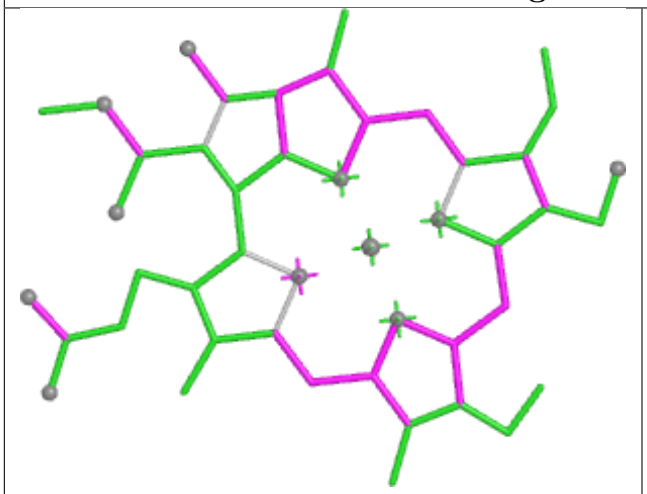


Rings

Ligand CHL 5 606



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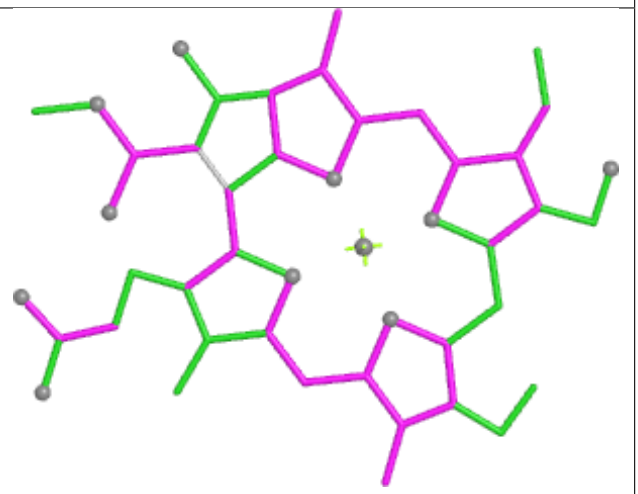
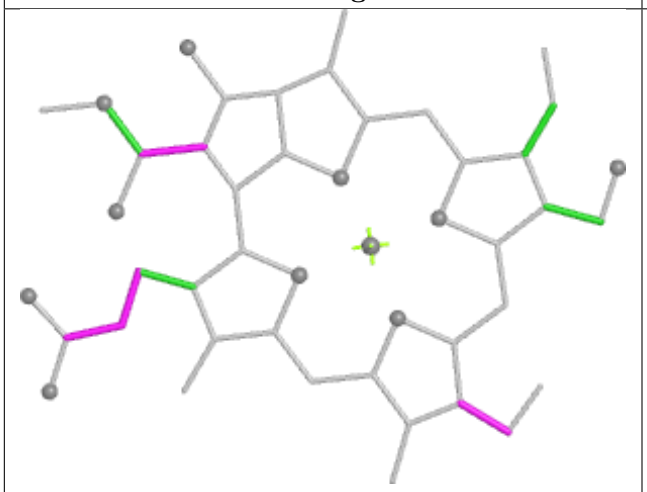


Bond angles



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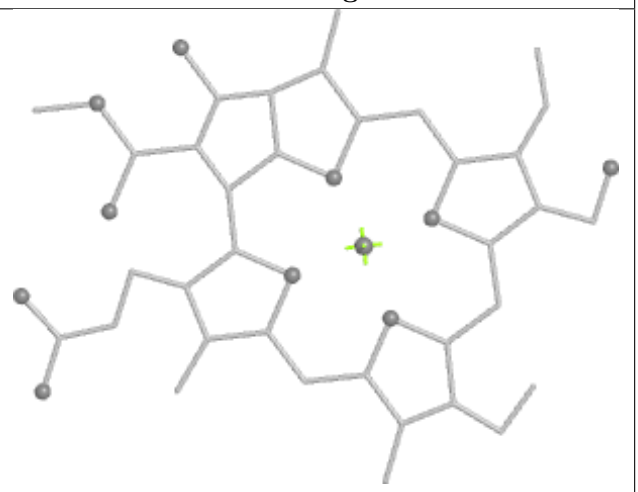
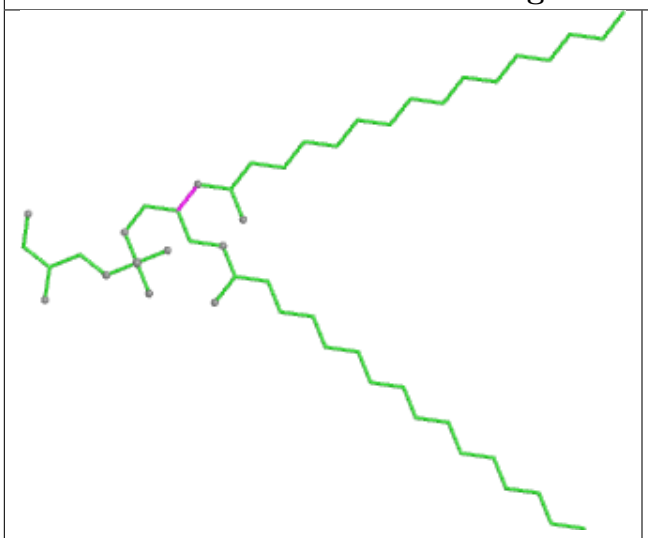


Rings

Ligand LHG v 621



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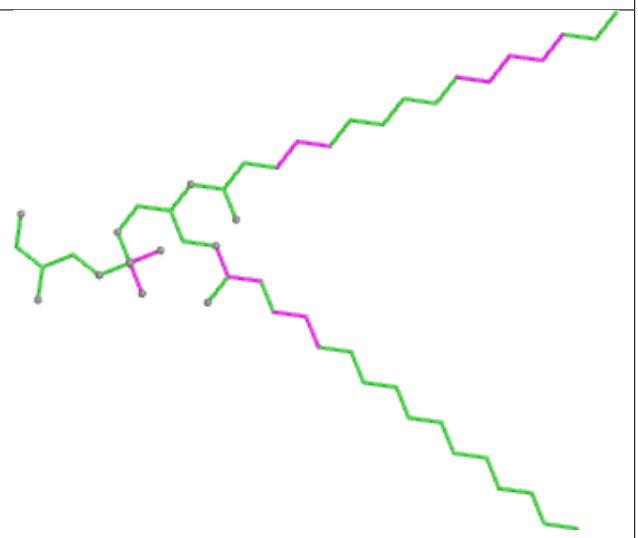
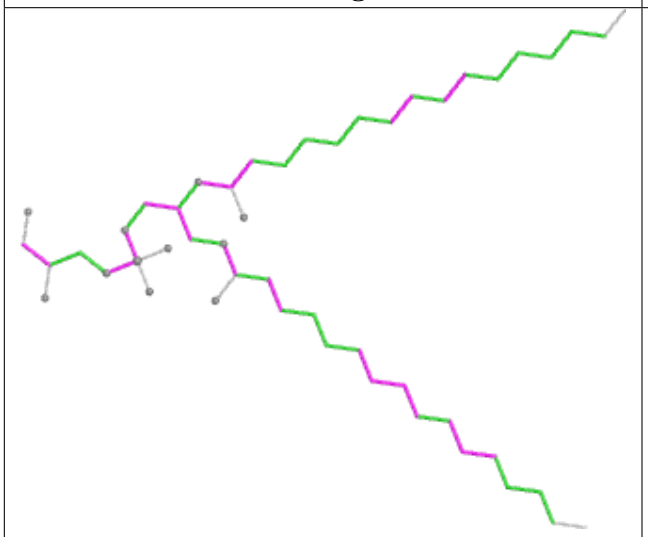
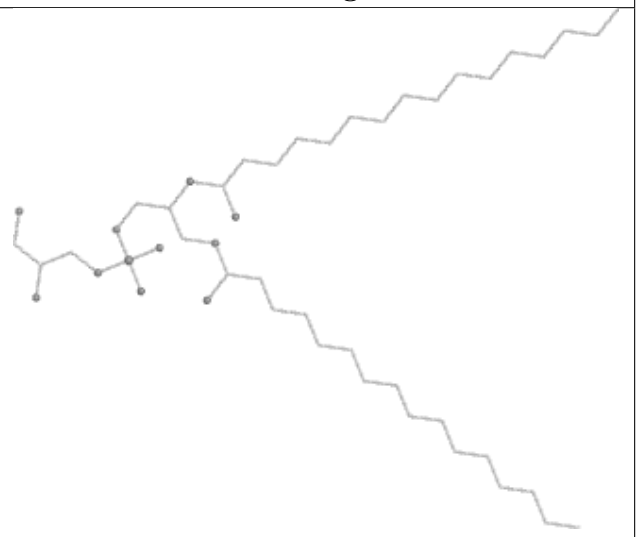


Bond angles

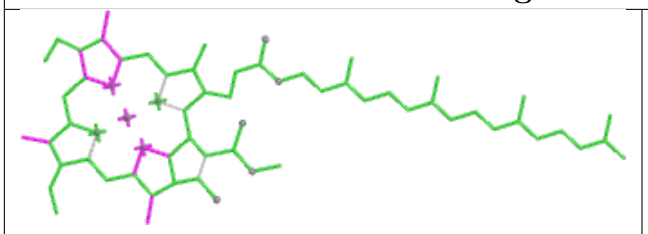


Torsions



Rings

Ligand CLA BF 503



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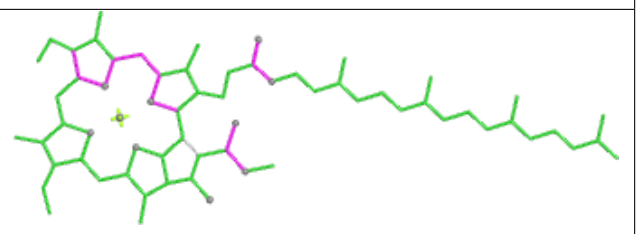
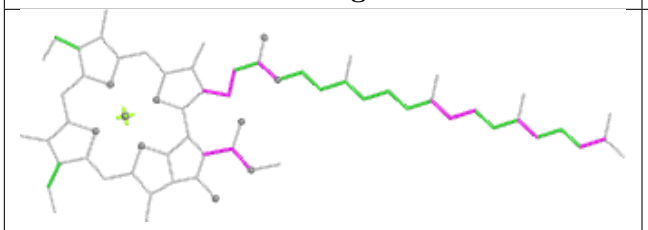


Bond angles



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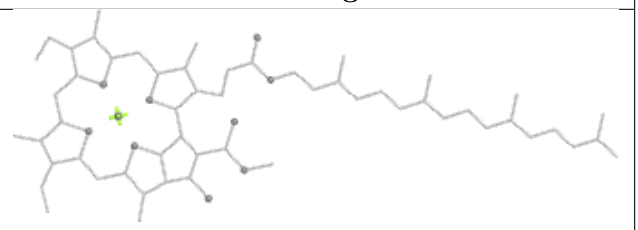
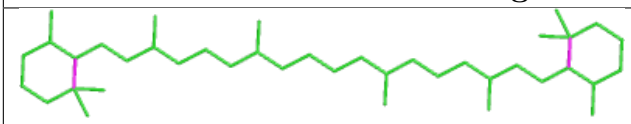


Rings

Ligand BCR BE 618



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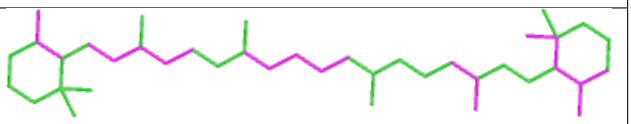
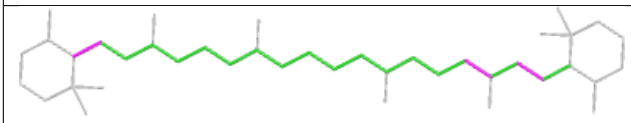


Bond angles



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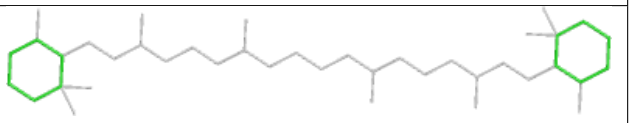
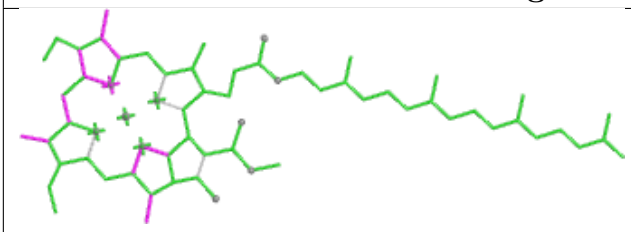


Rings

Ligand CLA b 616



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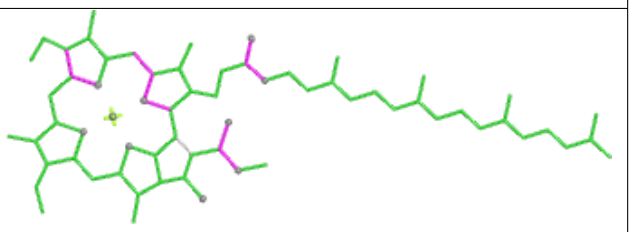

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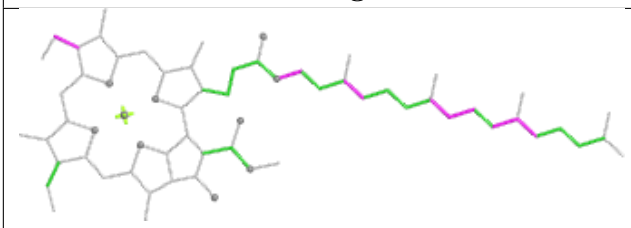

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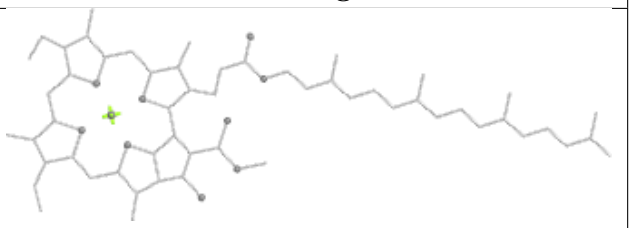
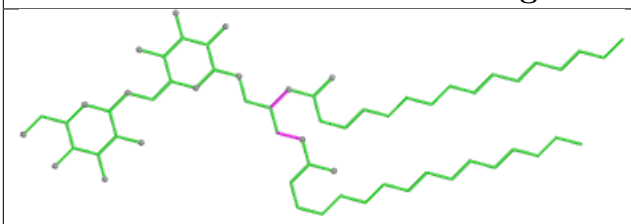


Rings

Ligand DGD C 517



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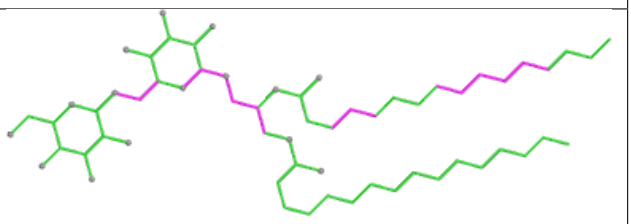
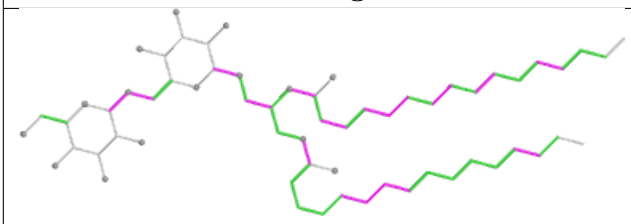


Bond angles



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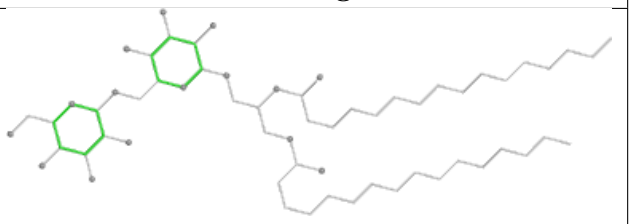
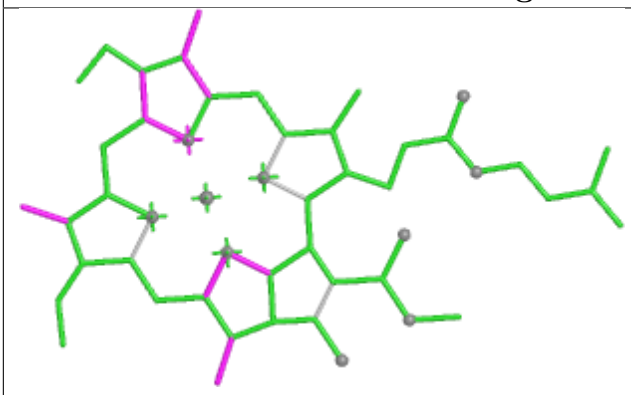


Rings

Ligand CLA Ba 305



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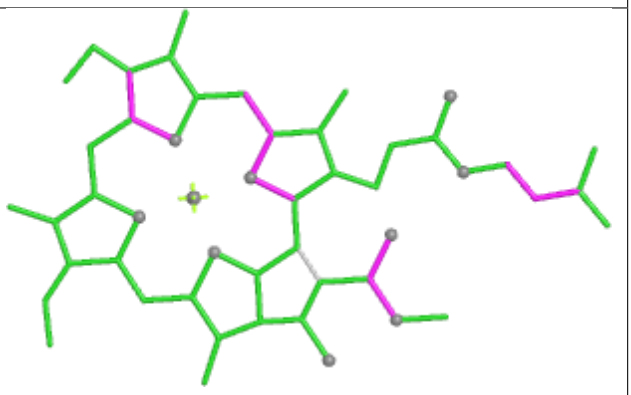
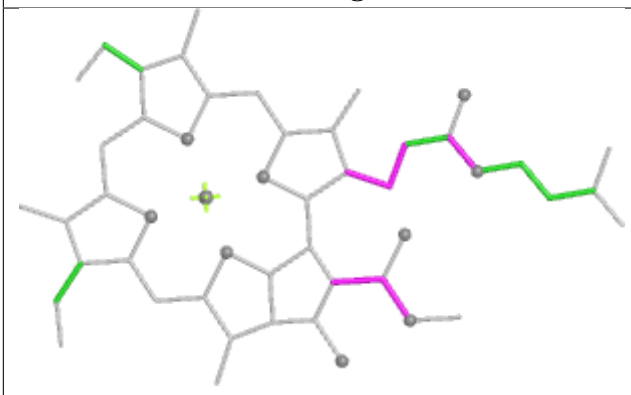


Bond angles



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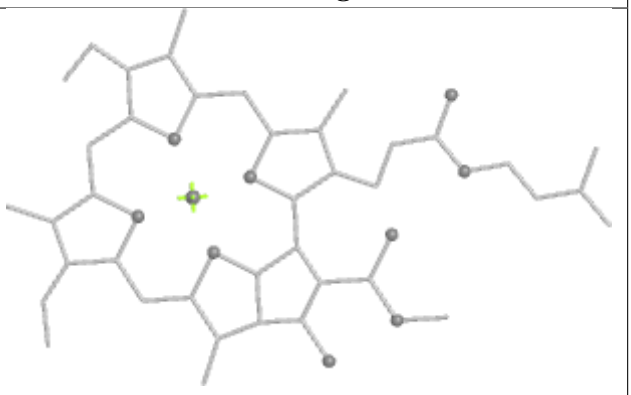
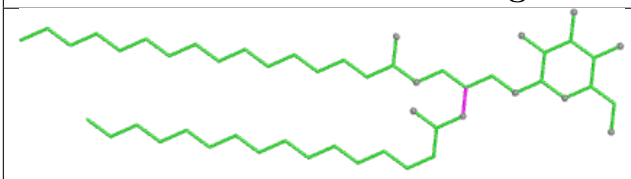


Rings

Ligand LMG BF 519



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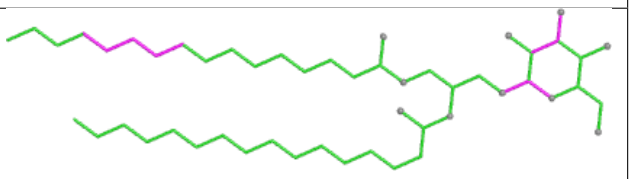
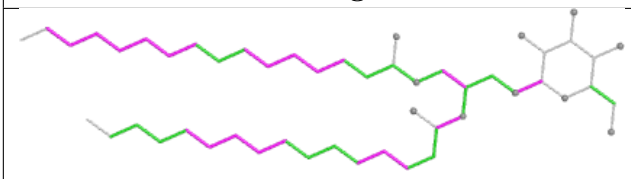


Bond angles



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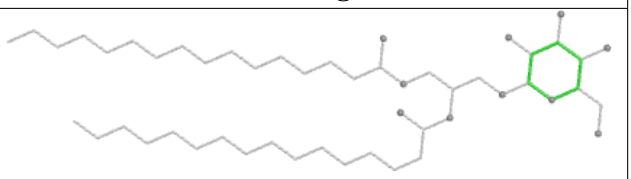
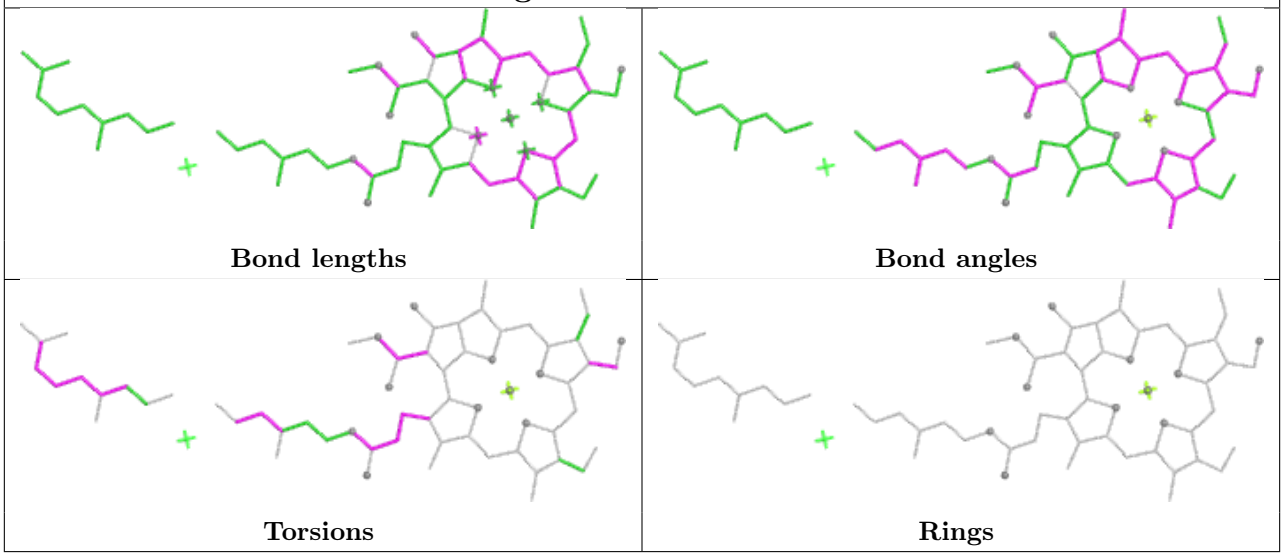
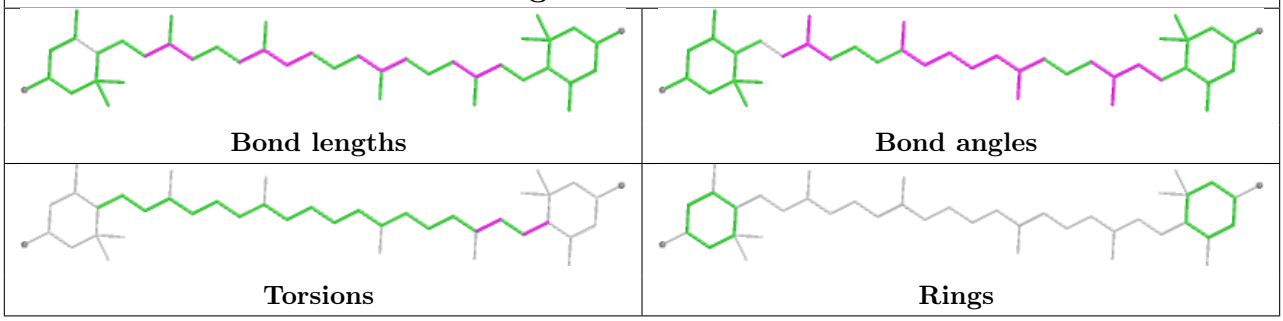


Rings

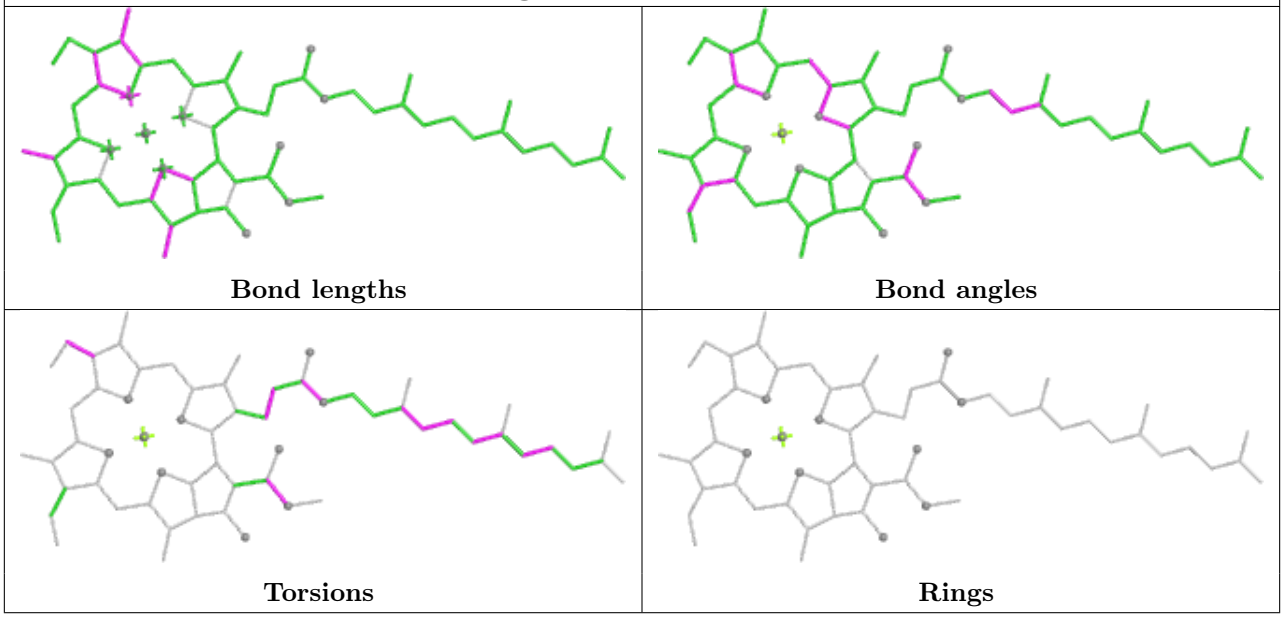
Ligand CHL Au 608

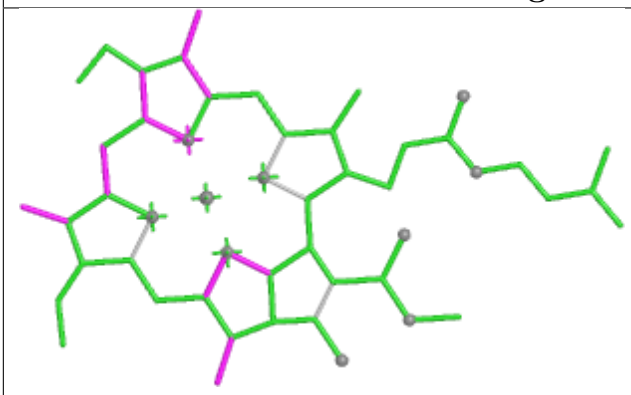
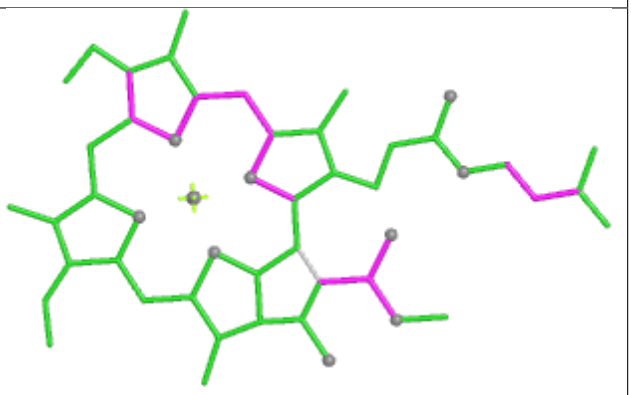
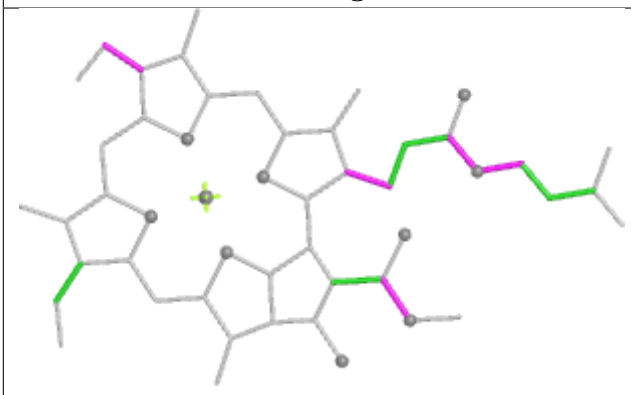
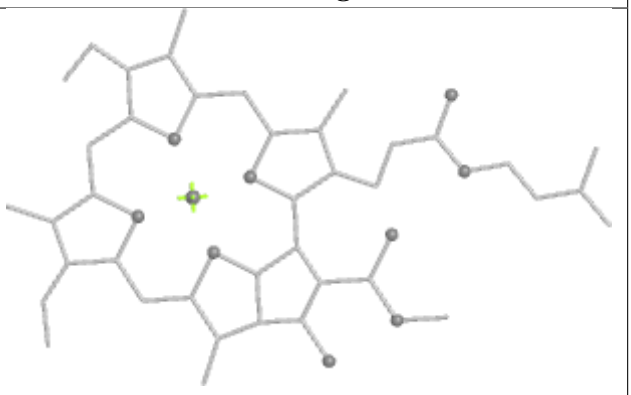


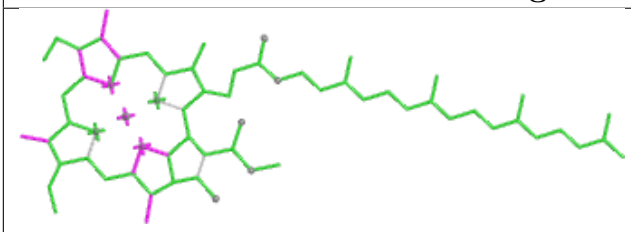
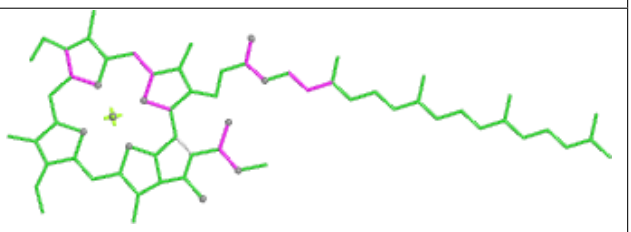
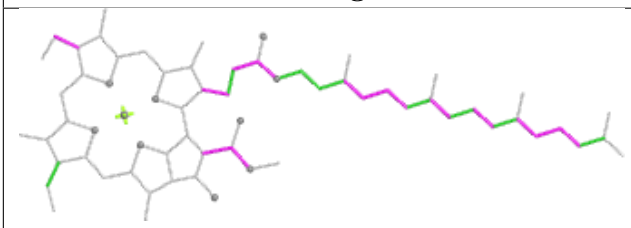
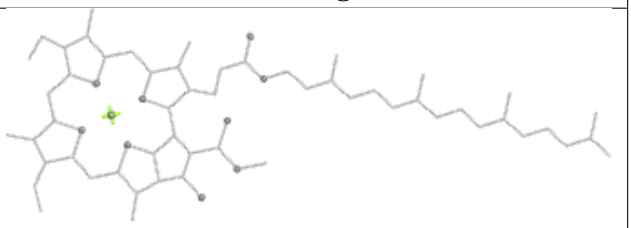
Ligand LUT 6 615



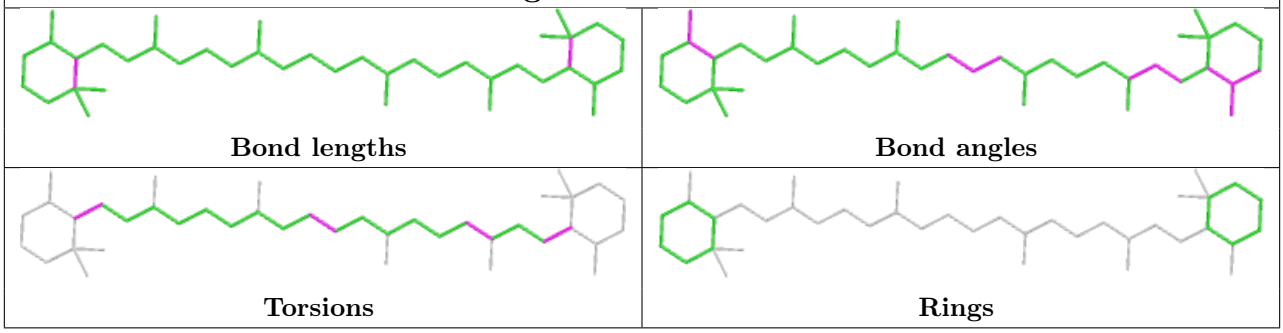
Ligand CLA A2 613



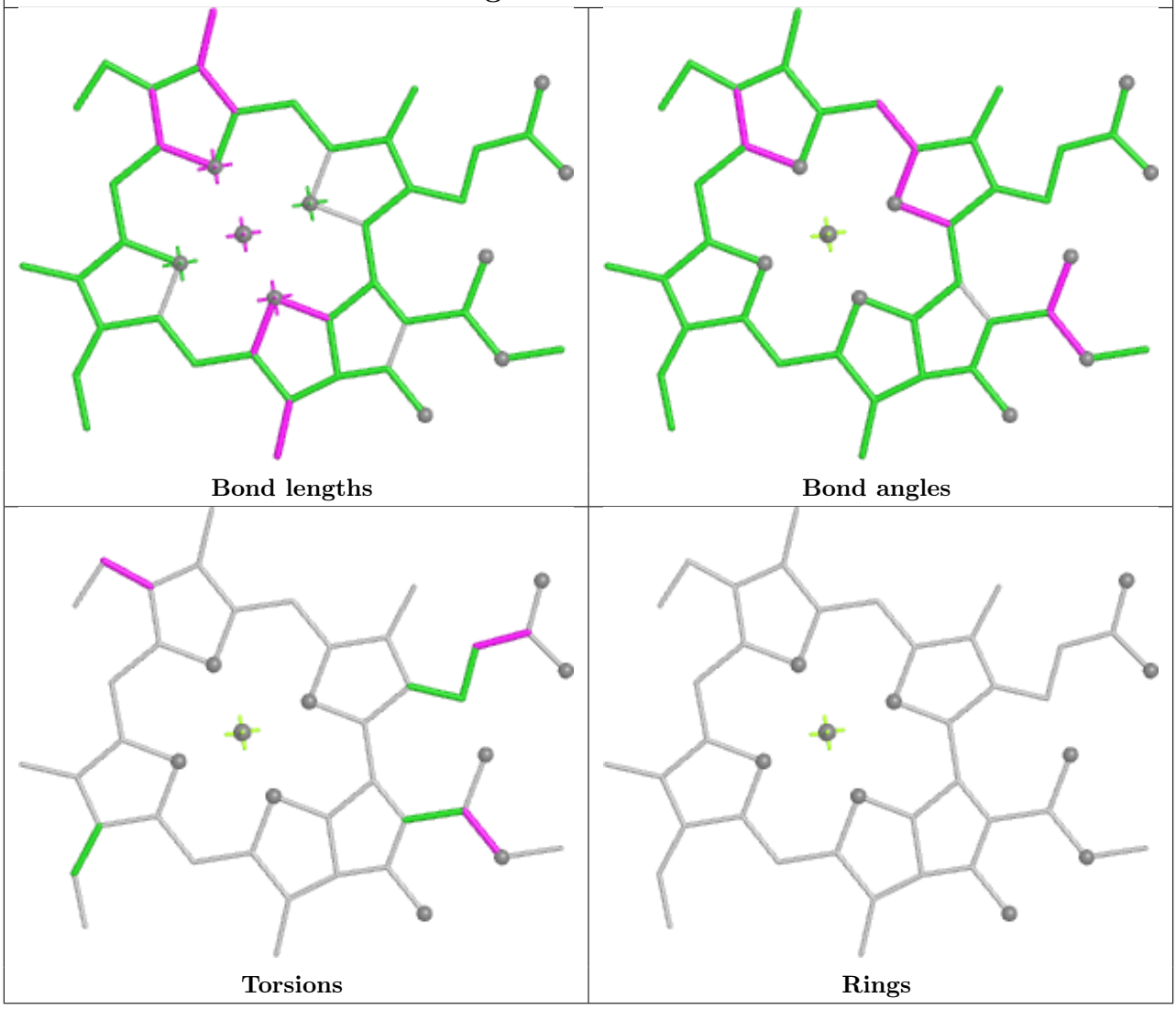
Ligand CLA a 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

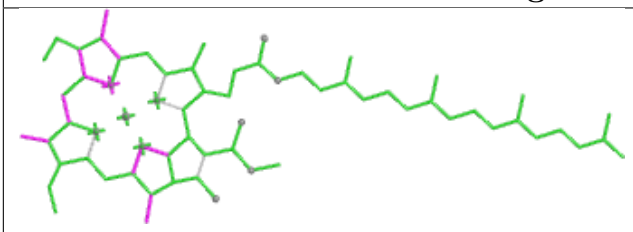
Ligand BCR B 619



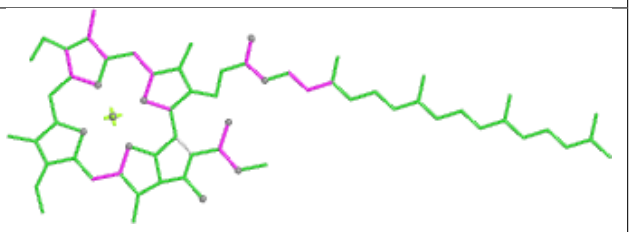
Ligand CLA 8 302



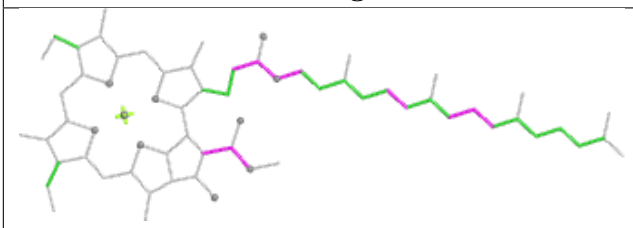
Ligand CLA b 612



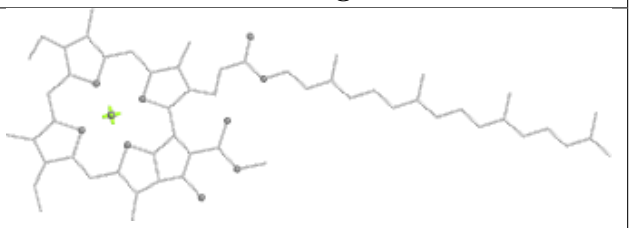
Bond lengths



Bond angles

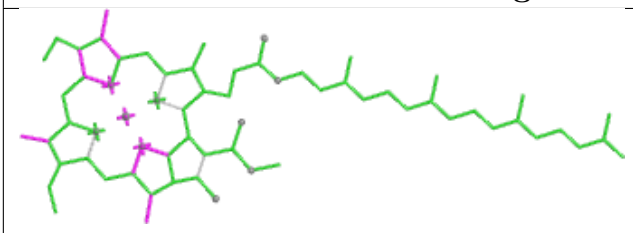


Torsions



Rings

Ligand CLA BF 504



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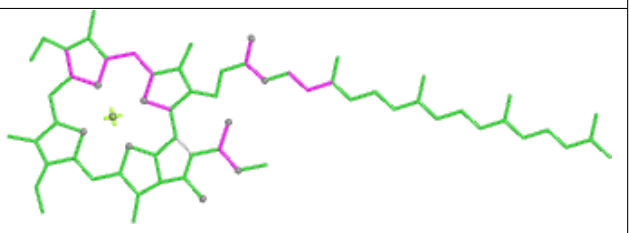
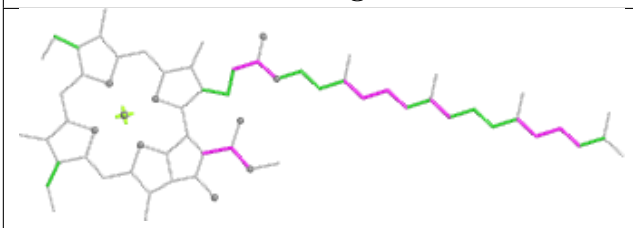


Bond angles



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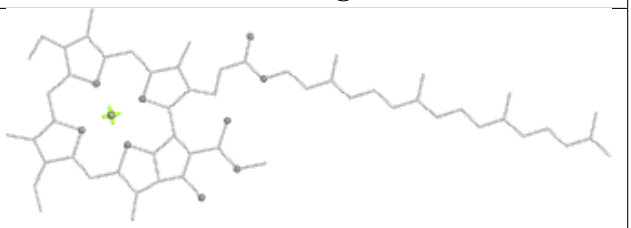
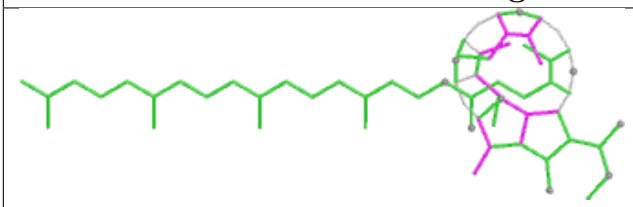
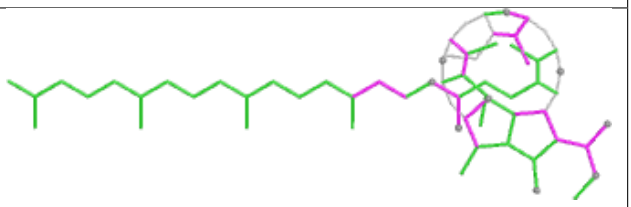


Rings

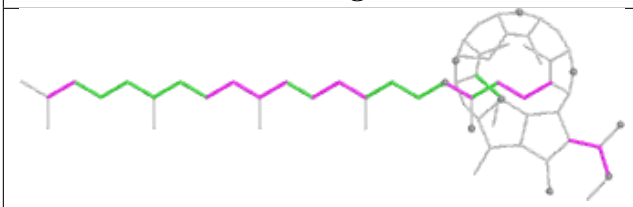
Ligand PHO BD 409



Bond lengths



Bond angles



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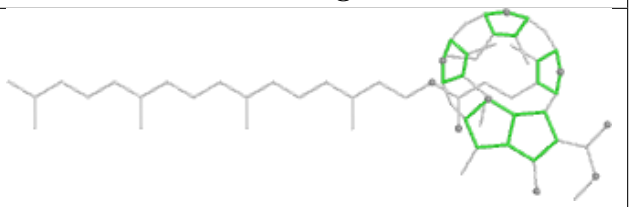
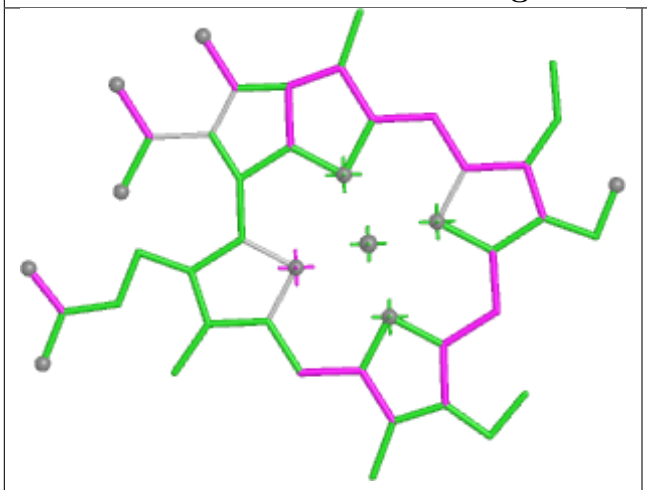
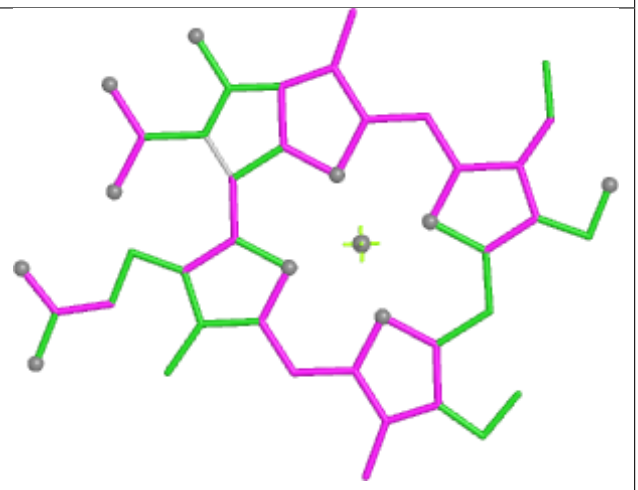


Rings

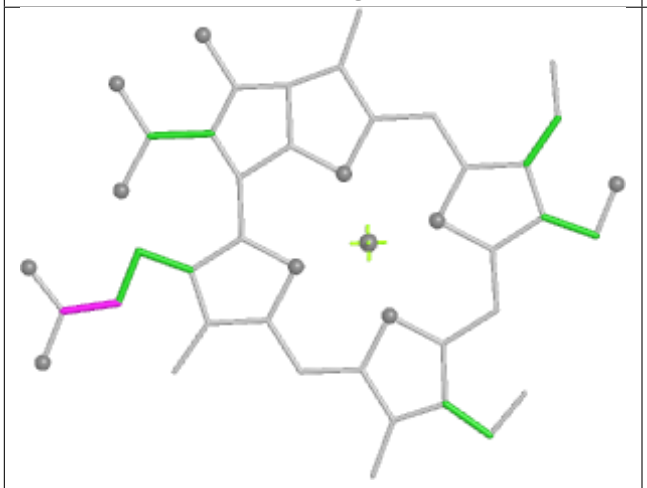
Ligand CHL BH 601



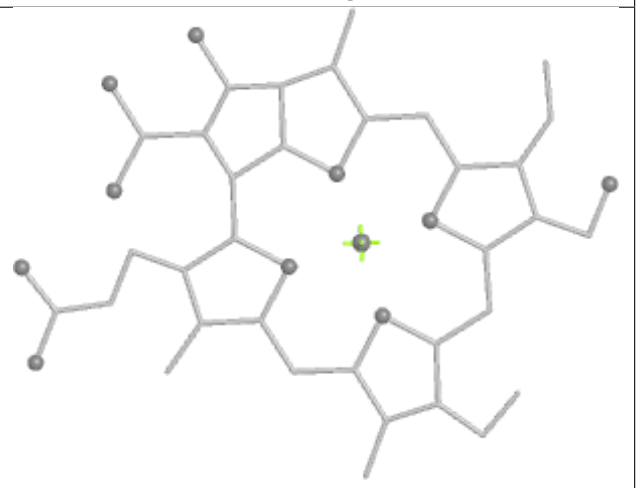
Bond lengths



Bond angles

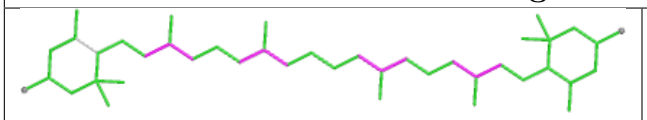


Torsions



Rings

Ligand LUT 0 616



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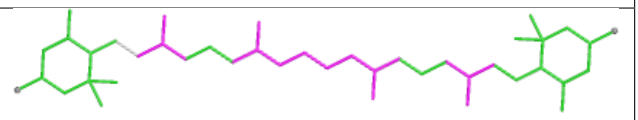
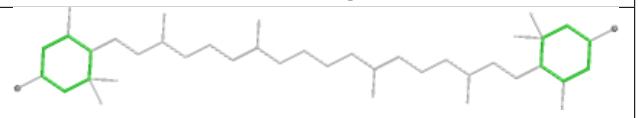
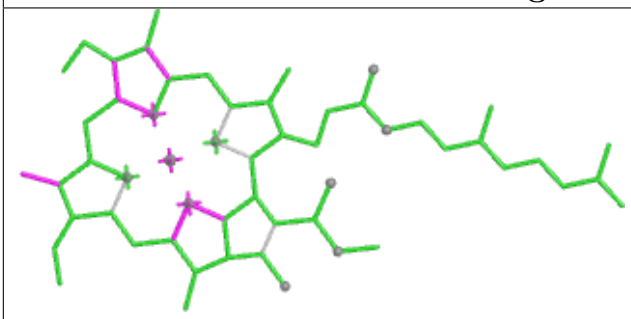
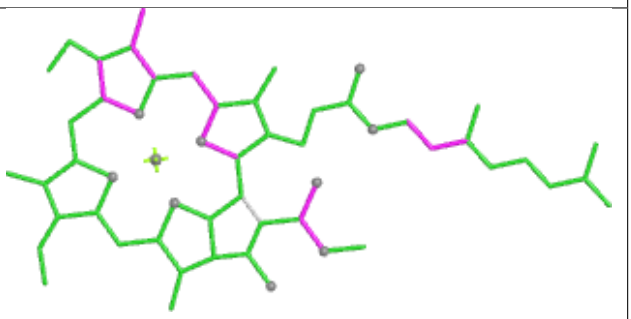
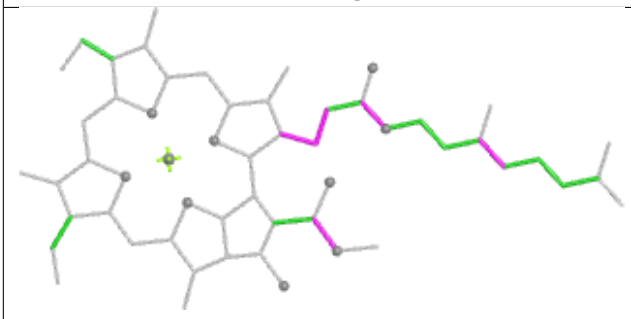
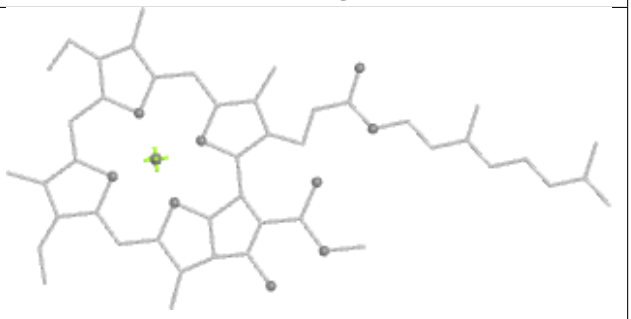


Bond angles

Torsions



Rings

Ligand CLA 5 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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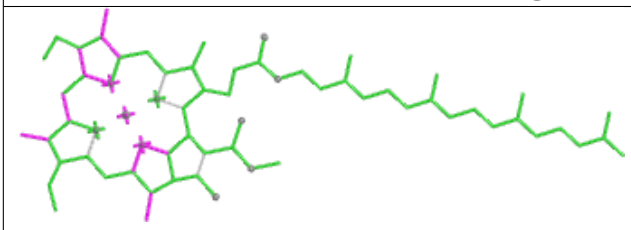
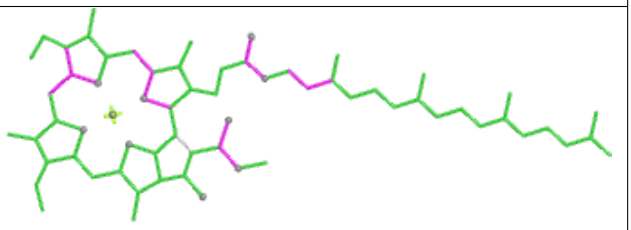
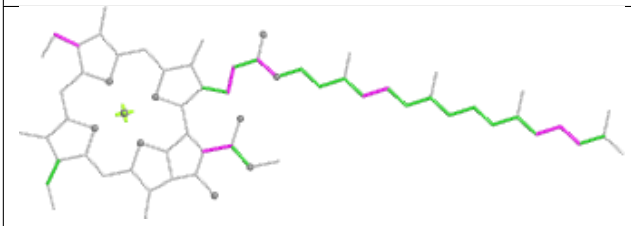
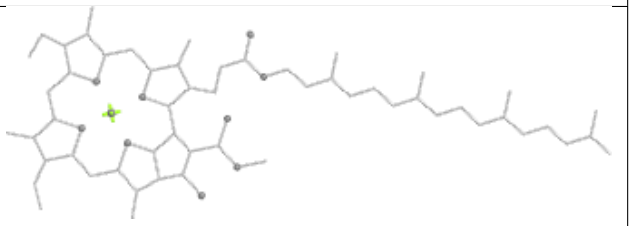
 Bond lengths	 Bond angles
 Torsions	 Rings

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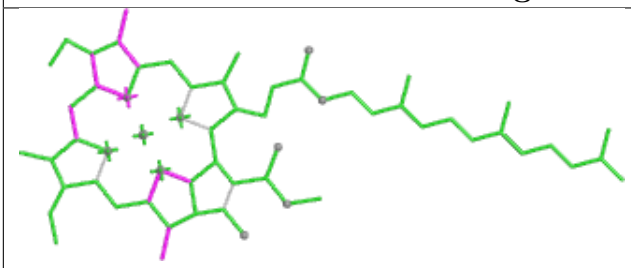
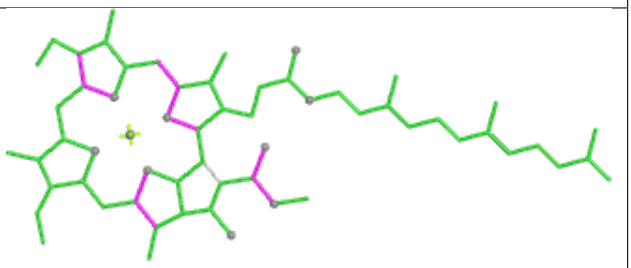
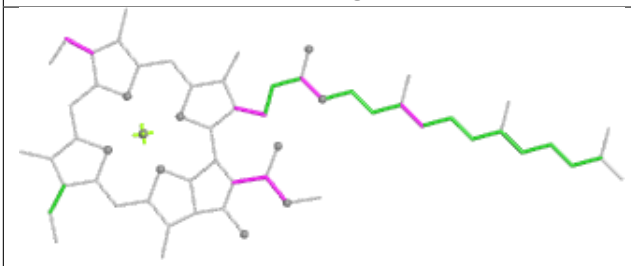
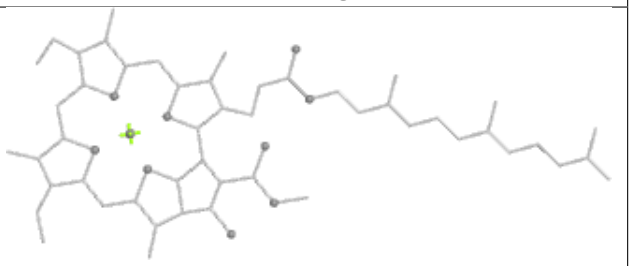
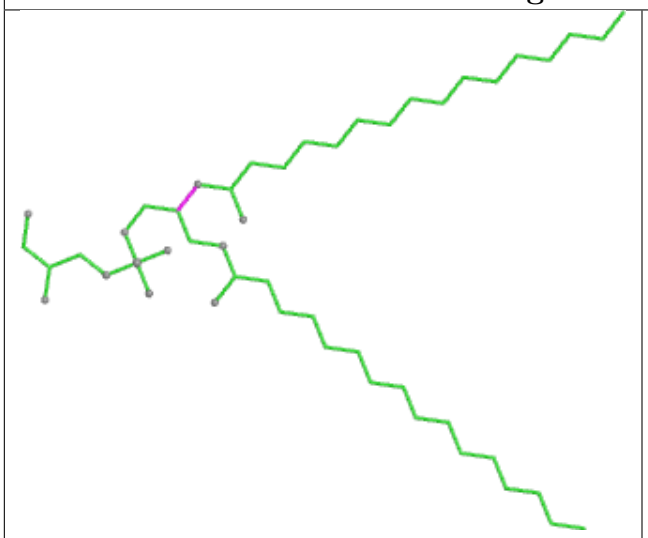
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG n 618



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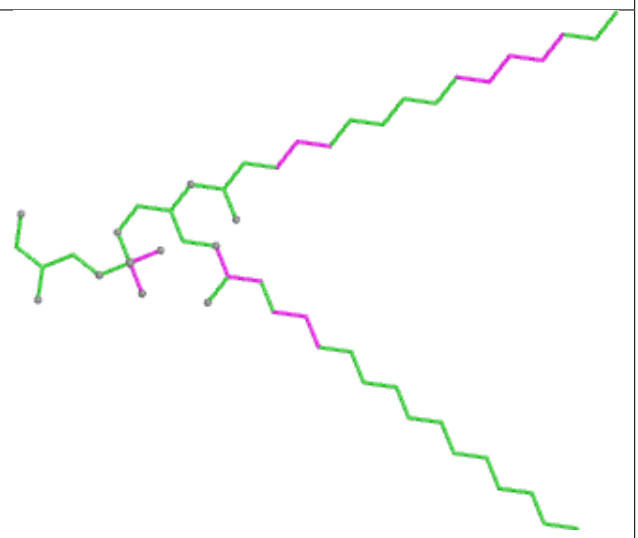

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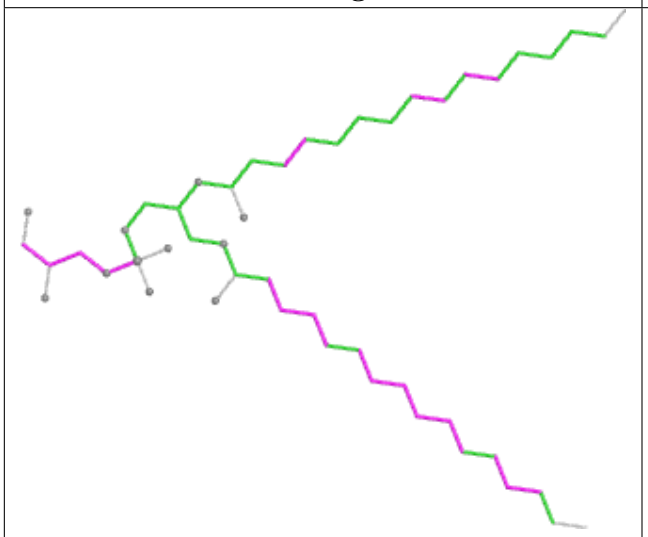

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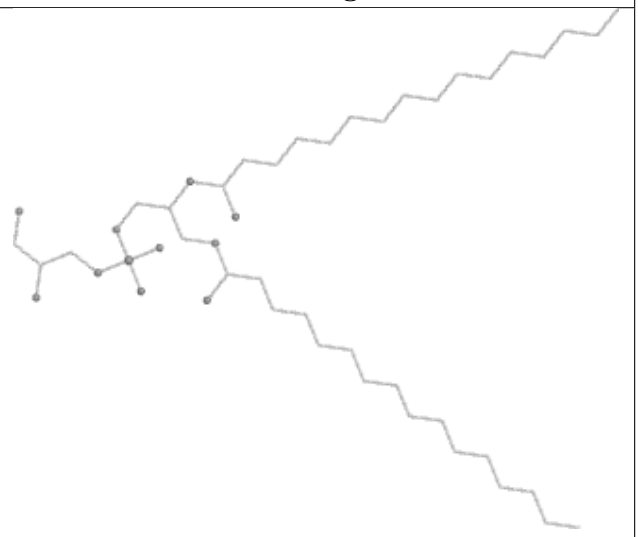
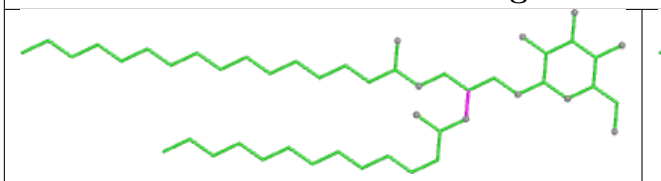


Rings

Ligand LMG BL 101



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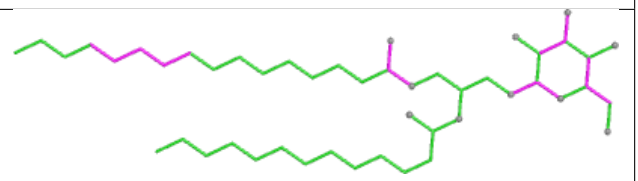

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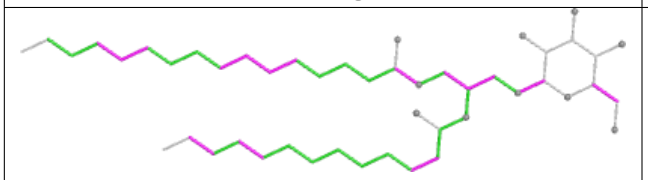

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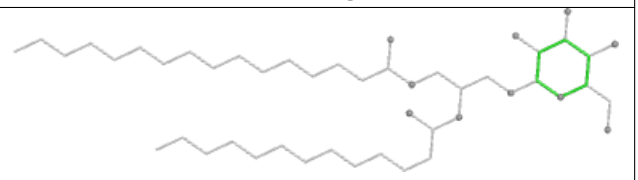

Rings

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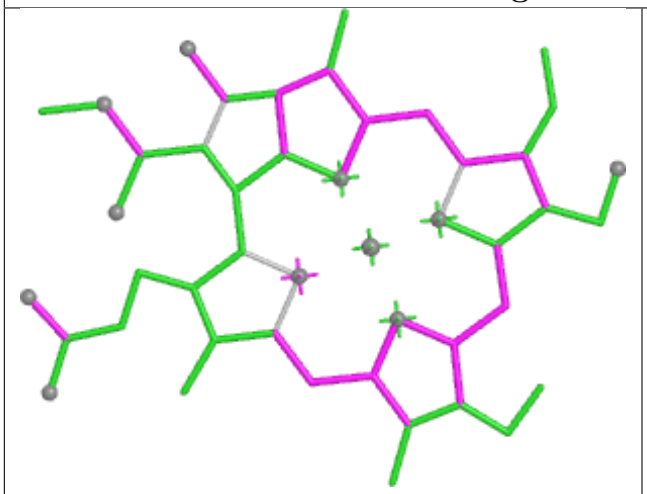

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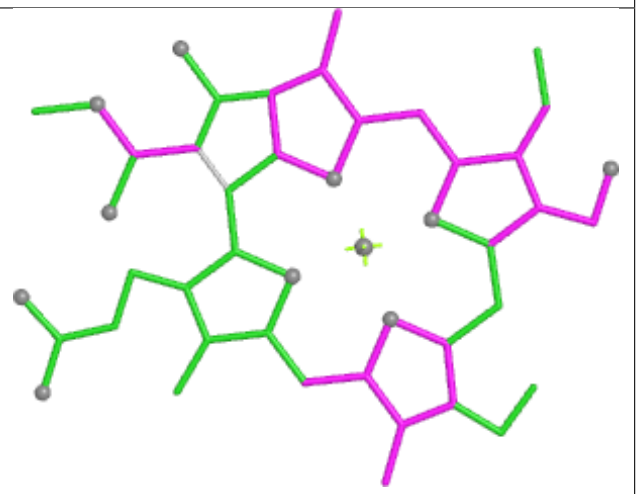
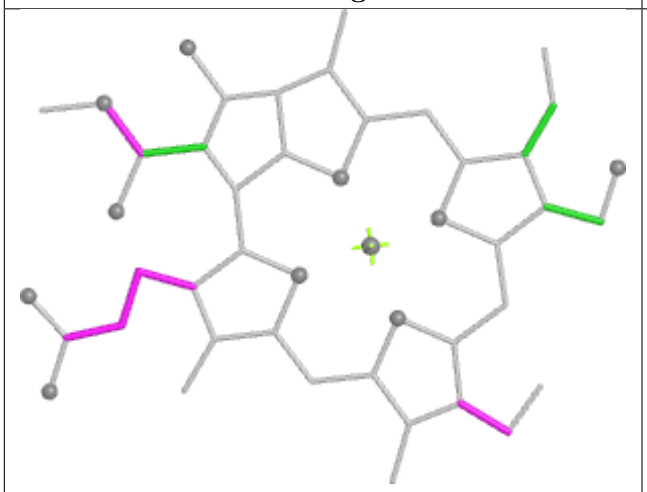


Bond angles



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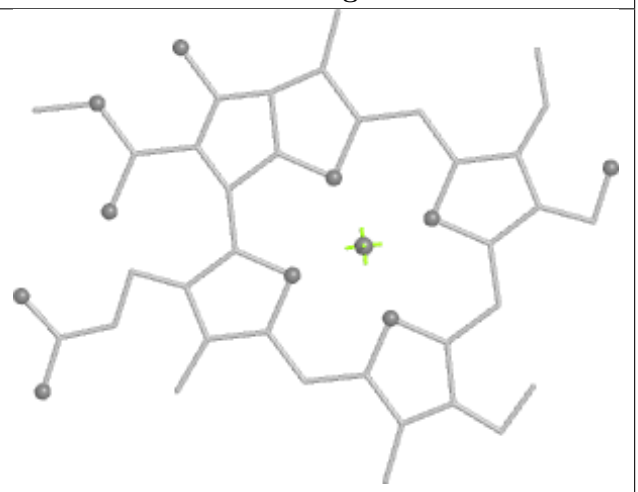
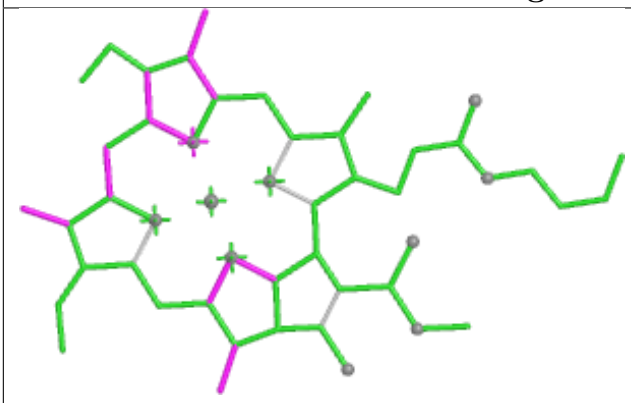
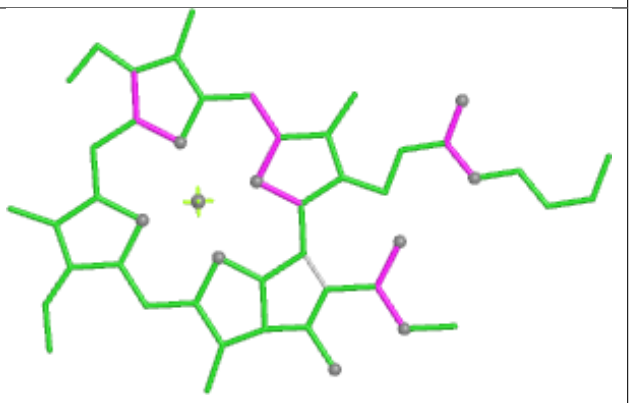
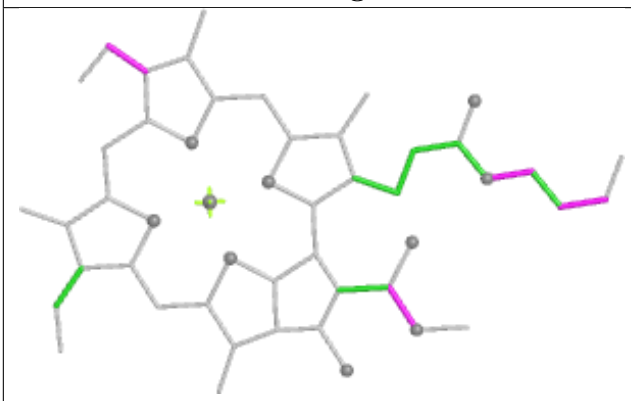
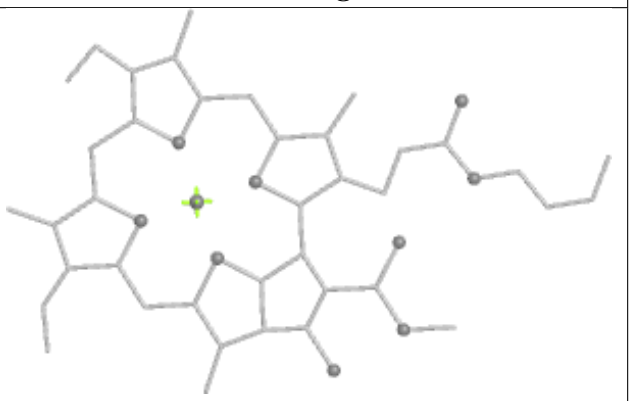


Rings

Ligand CLA S 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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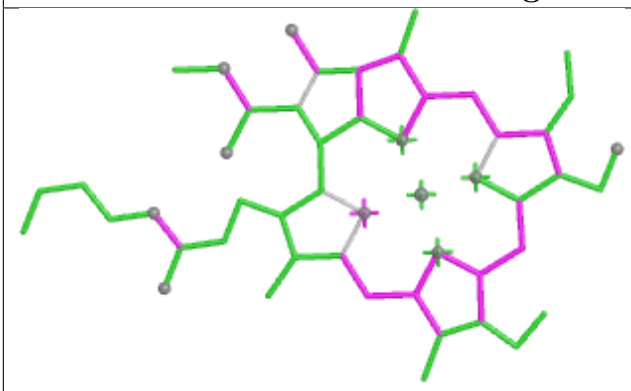

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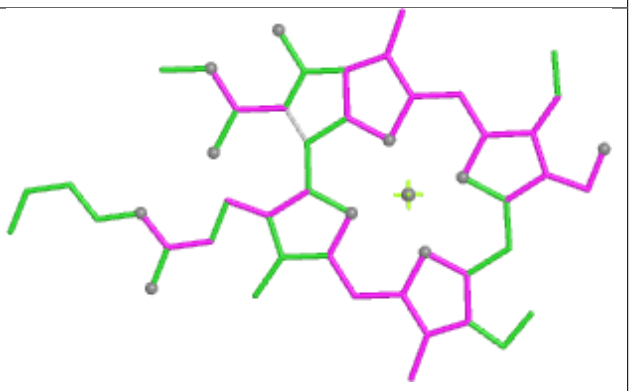
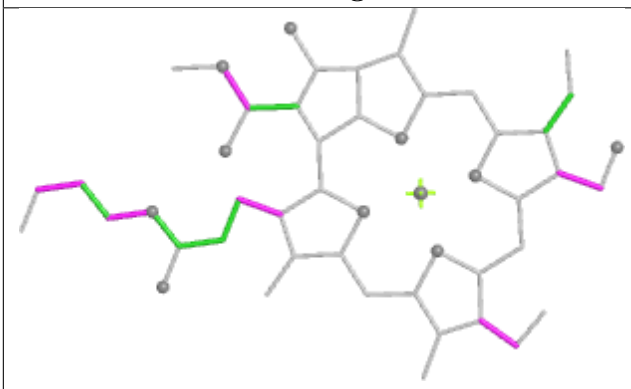


Bond angles



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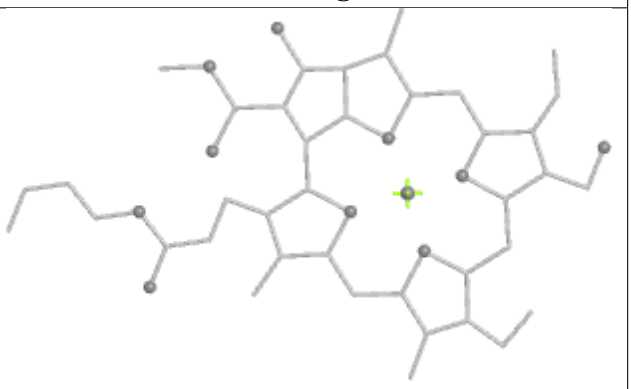

Rings

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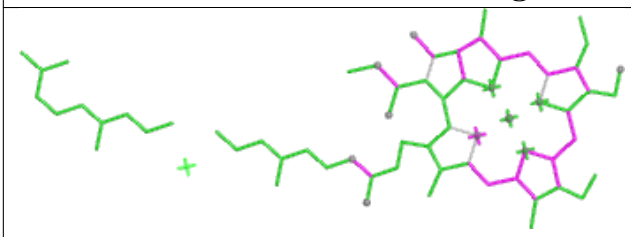

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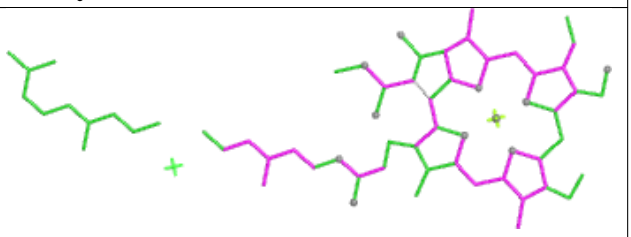

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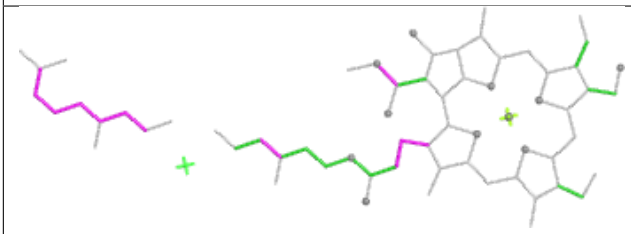

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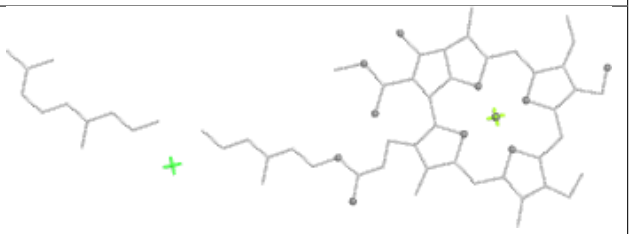

Rings

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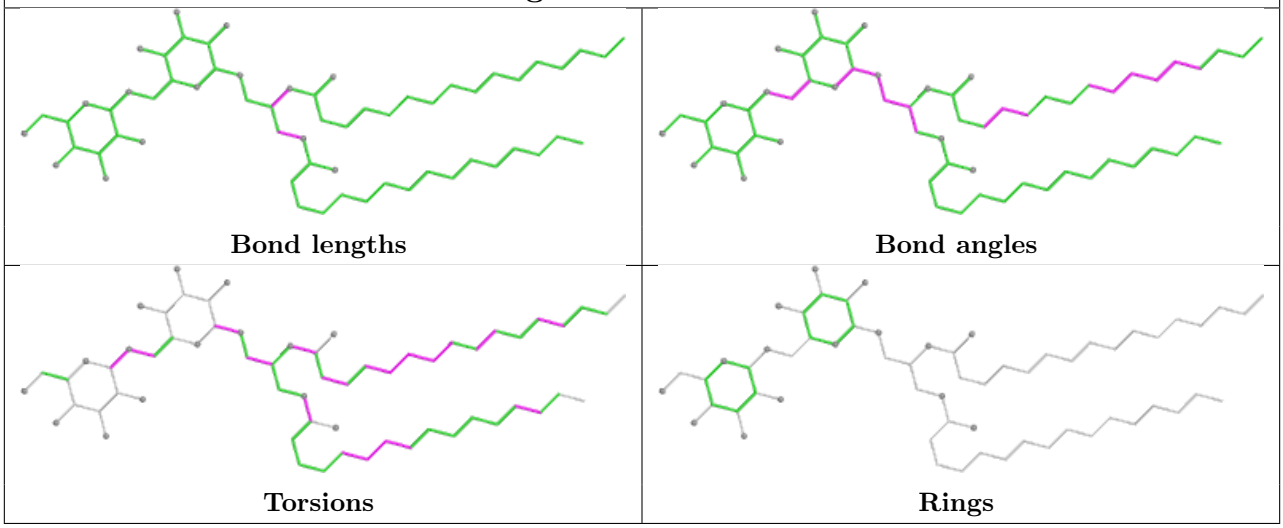

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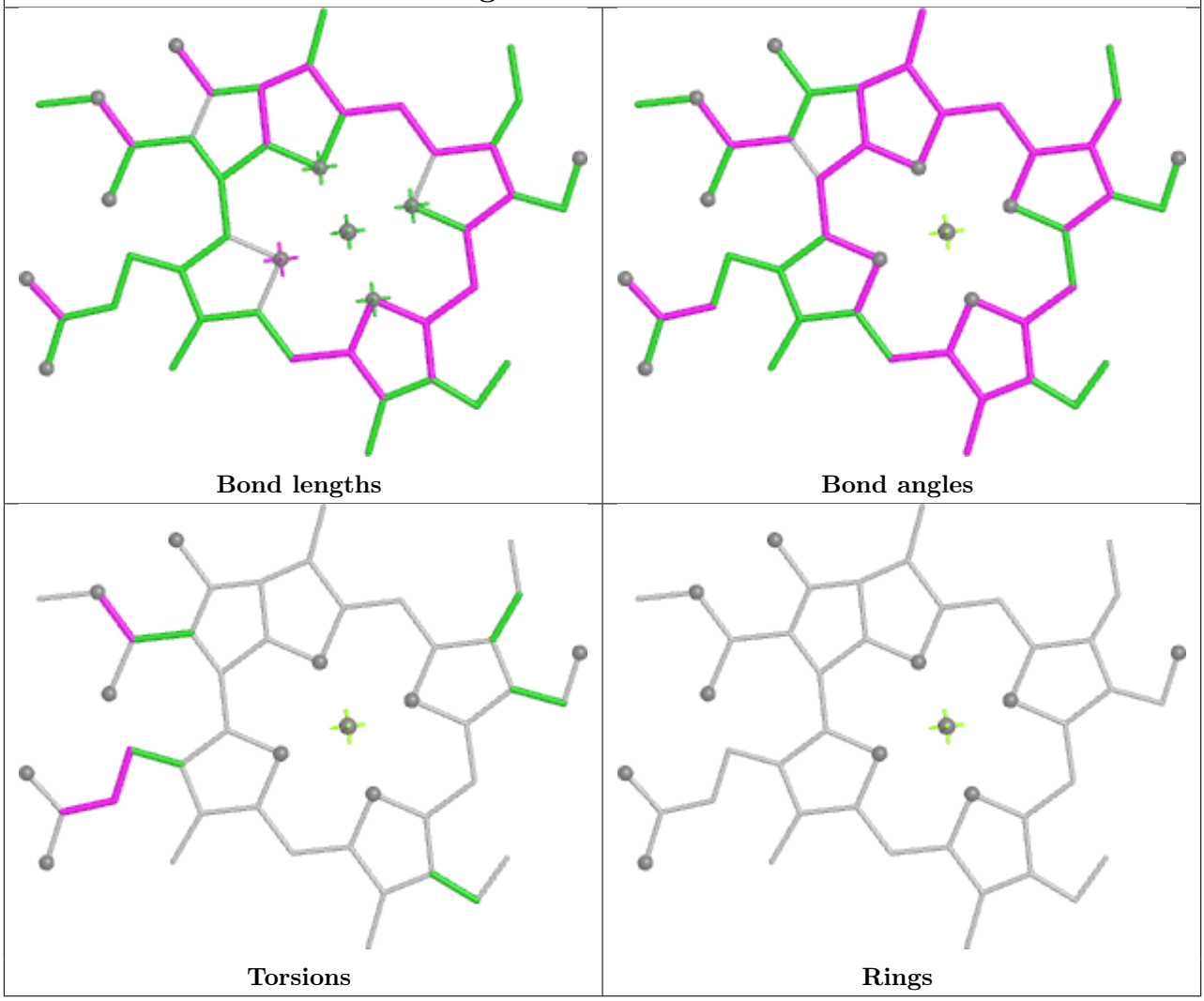

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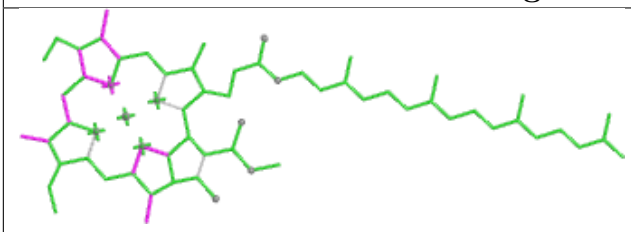

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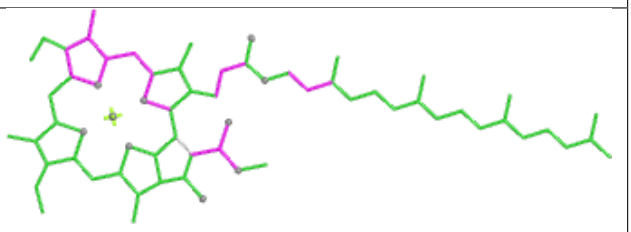

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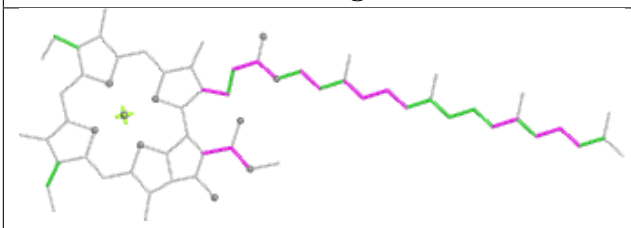

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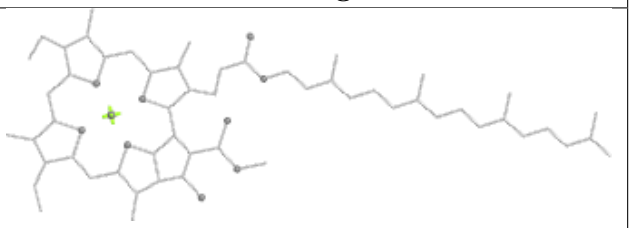

Rings

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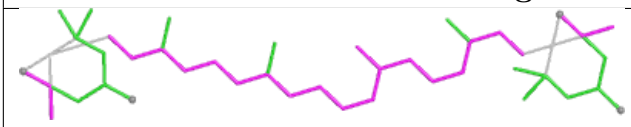
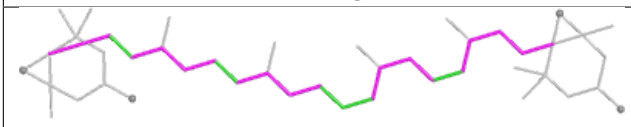


Bond lengths

Bond angles



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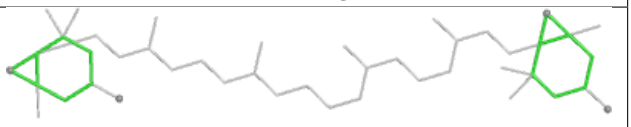


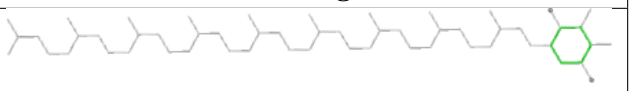
Rings

Ligand PL9 BG 403

Bond lengths

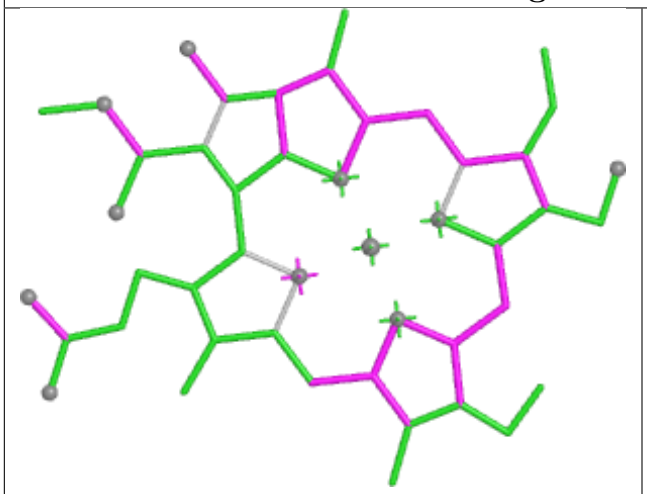
Bond angles

Torsions



Rings

Ligand CHL 0 605



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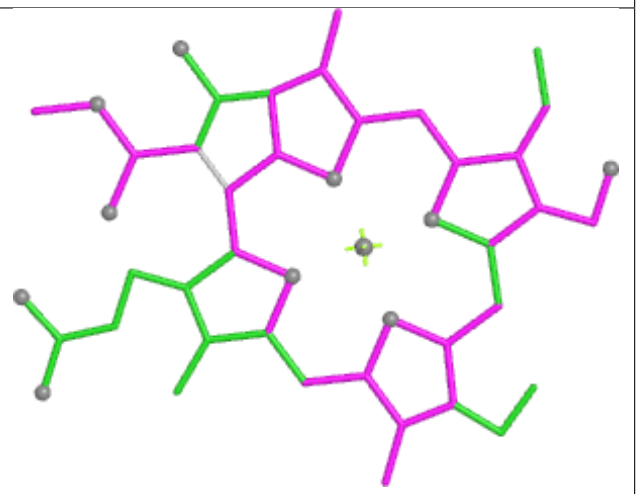
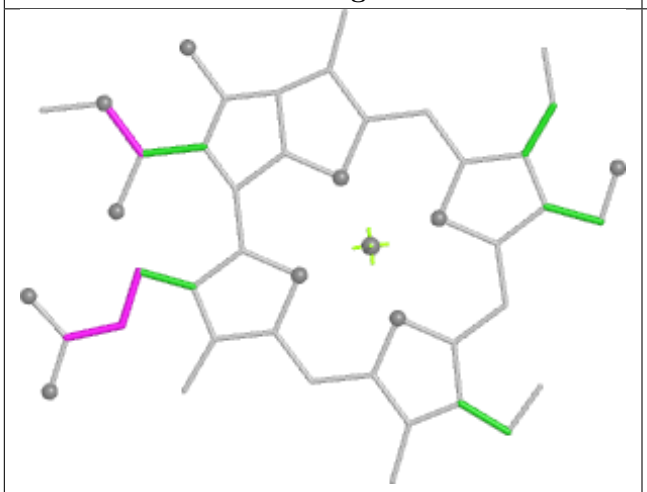


Bond angles



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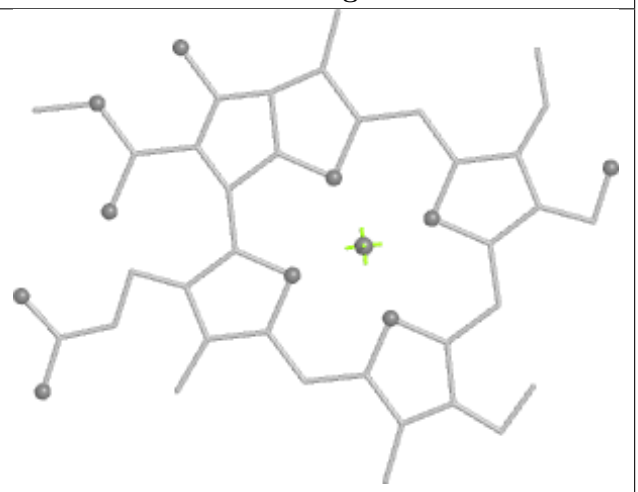

Rings

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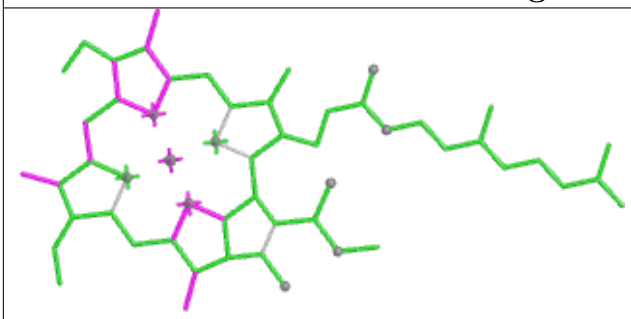
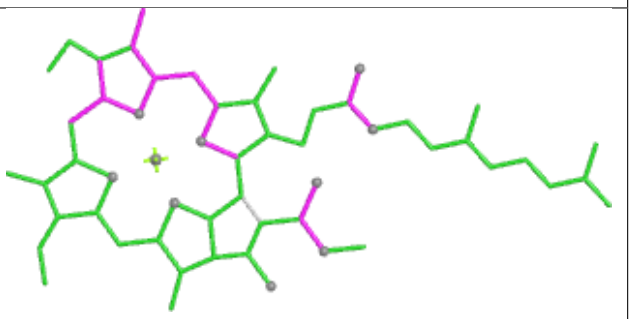
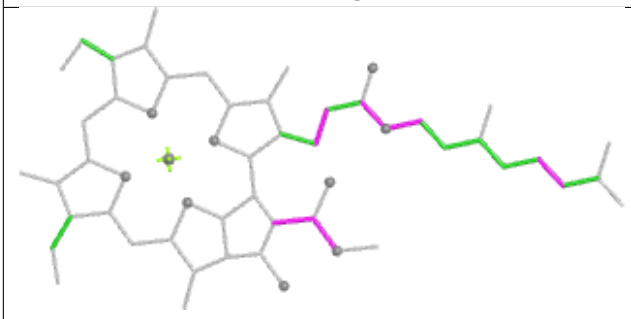
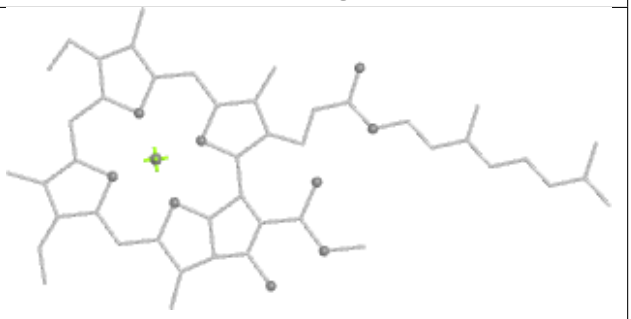
 Bond lengths	 Bond angles
 Torsions	 Rings

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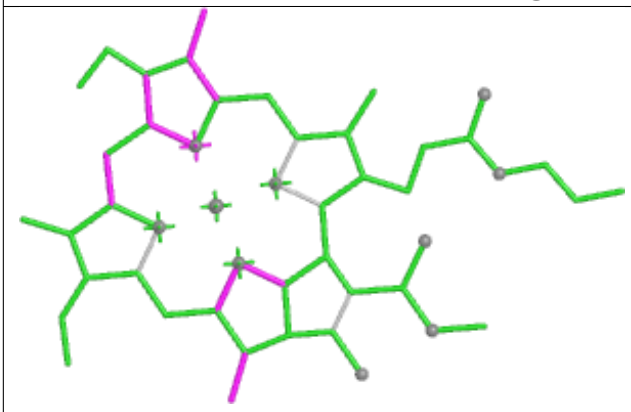
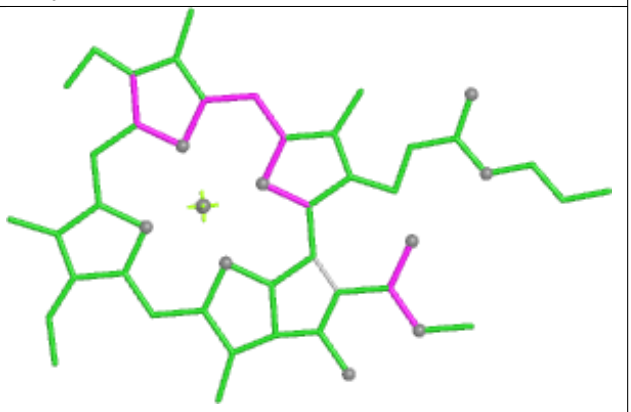
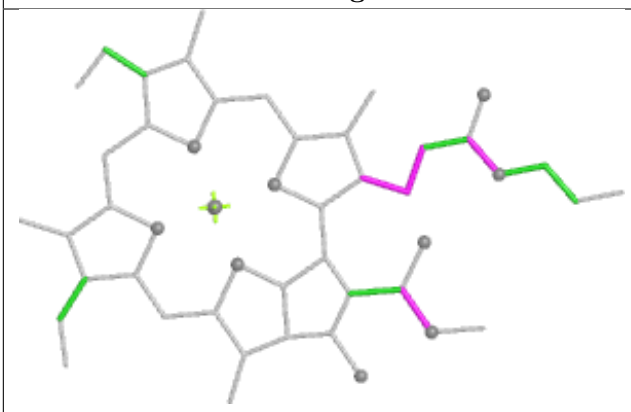
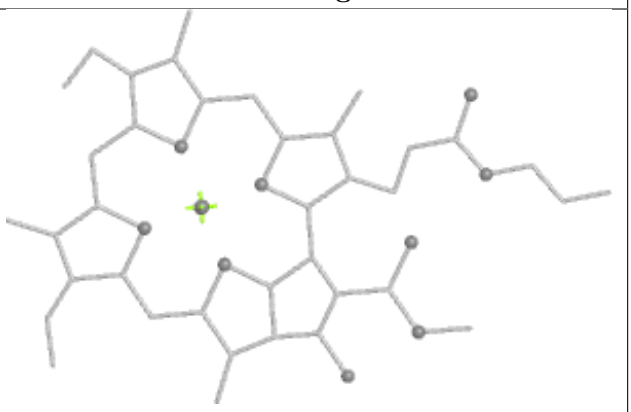
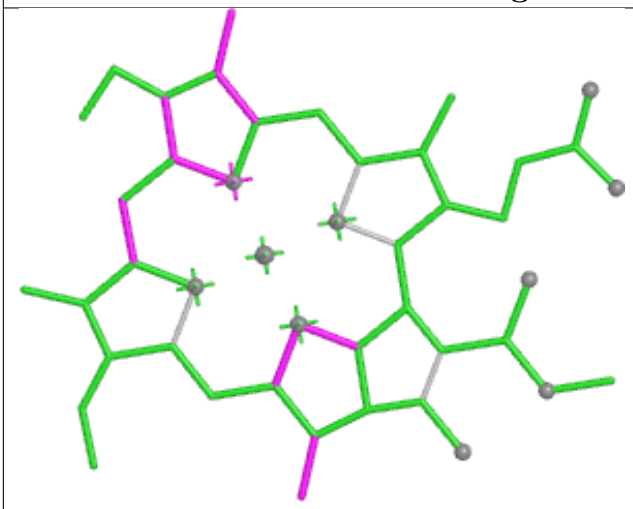
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AB 310



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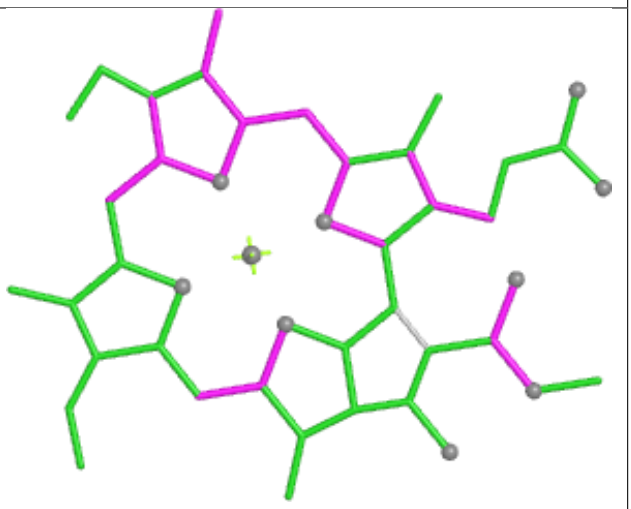

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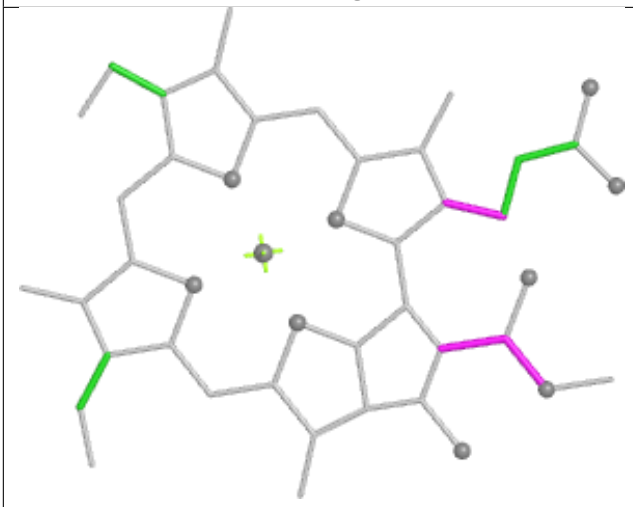

Torsions

Rings

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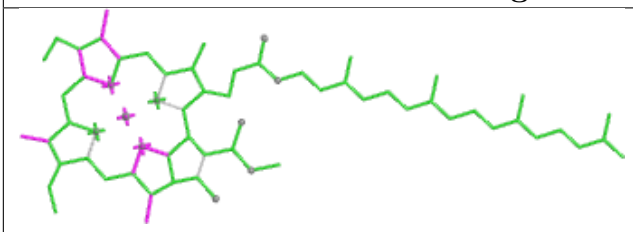

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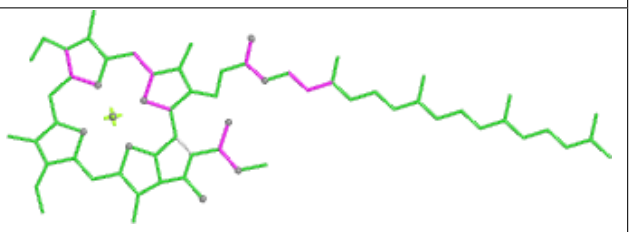

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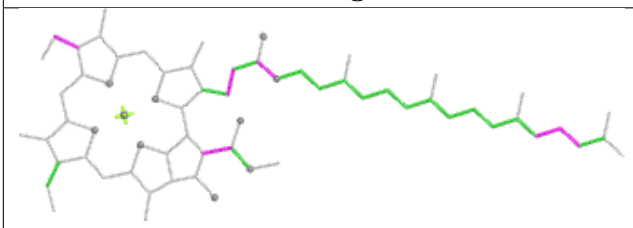

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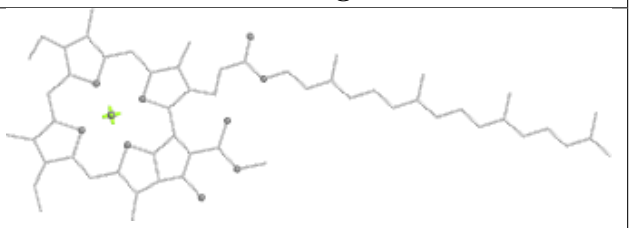

Rings

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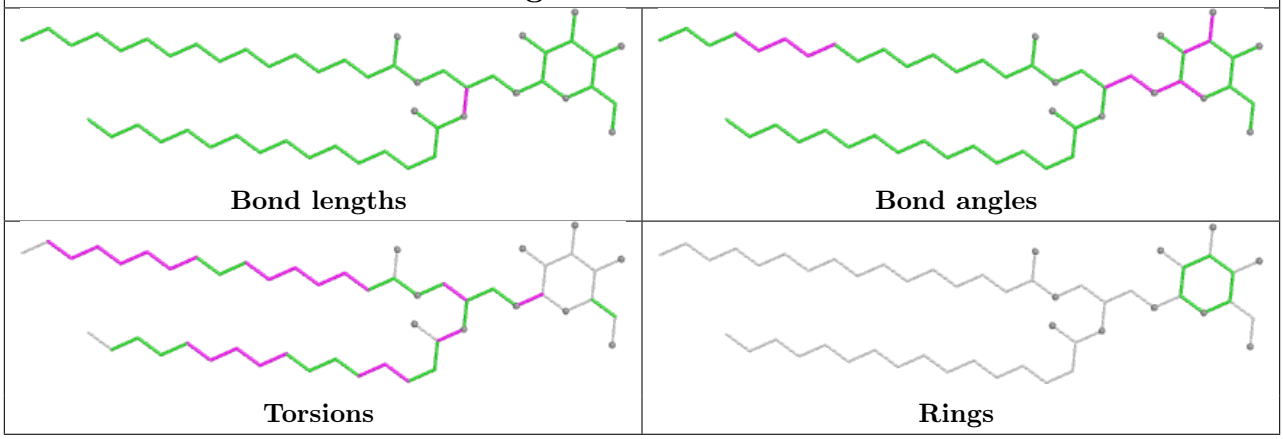

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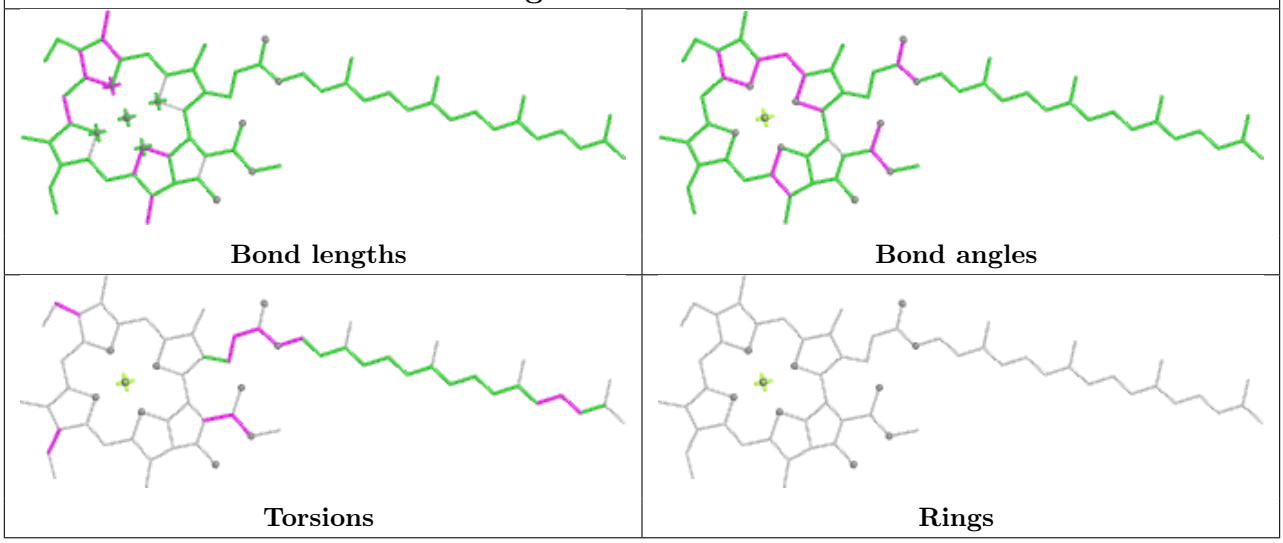

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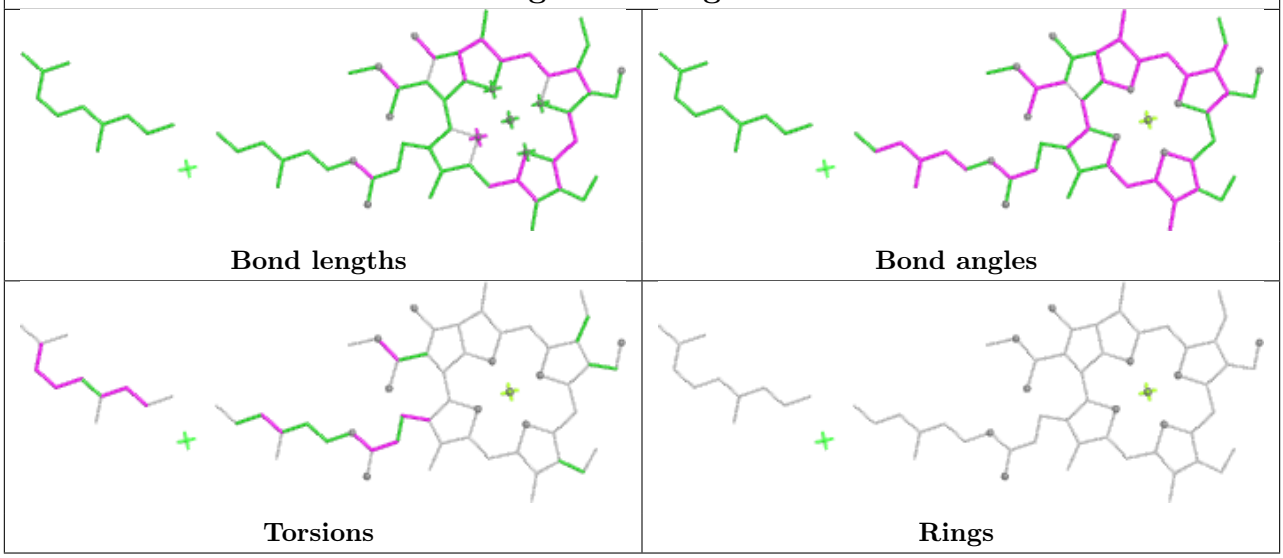

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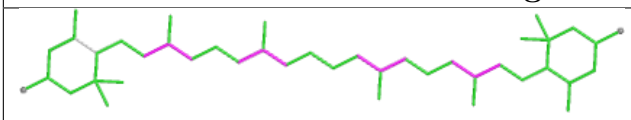
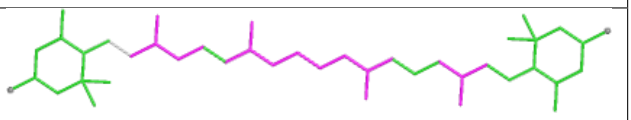
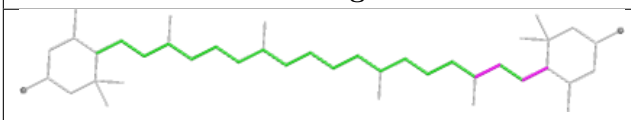
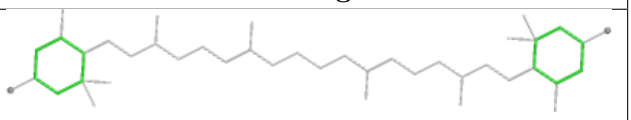
 Bond lengths	 Bond angles
 Torsions	 Rings

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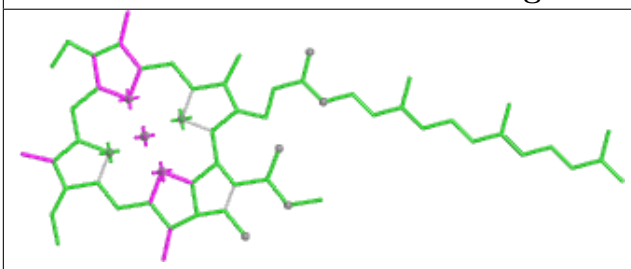
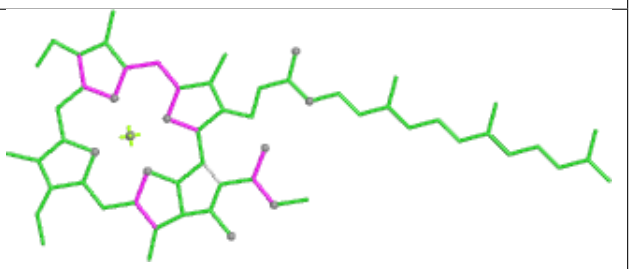
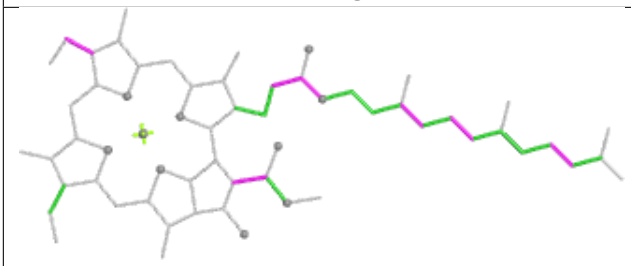
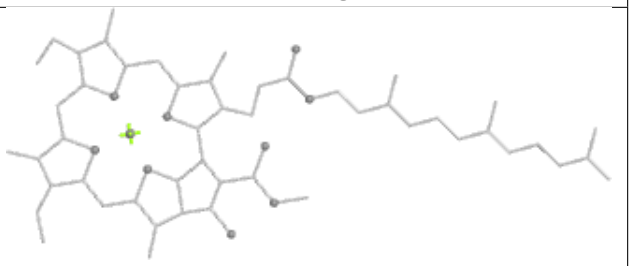
 Bond lengths	 Bond angles
 Torsions	 Rings

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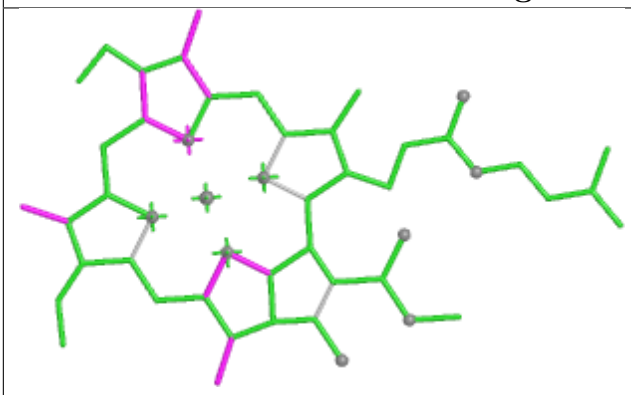
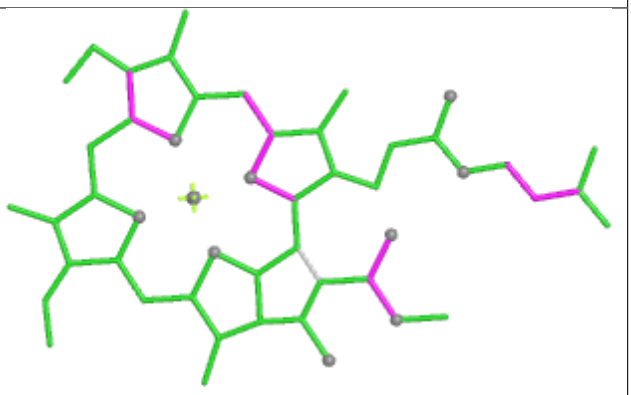
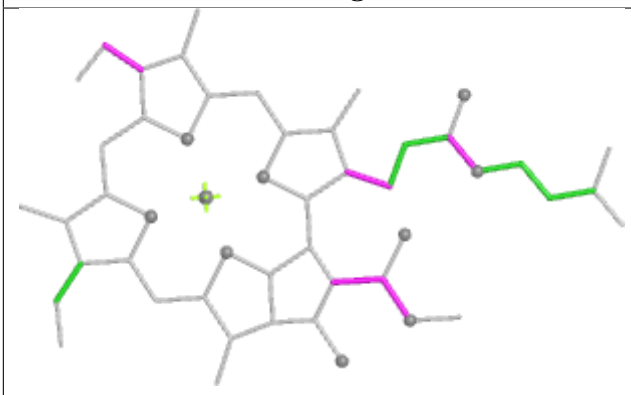
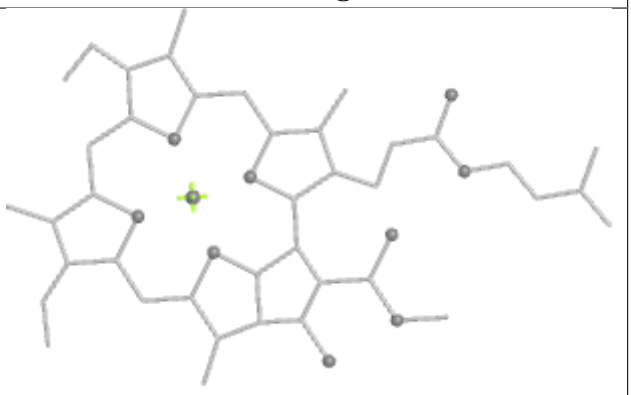
 Bond lengths	 Bond angles
 Torsions	 Rings

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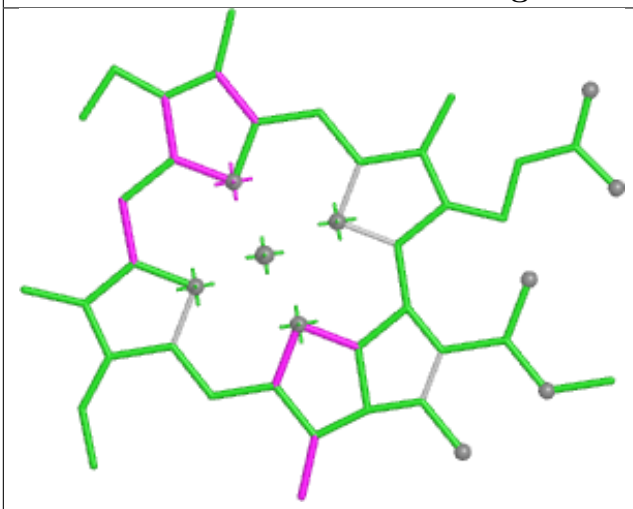

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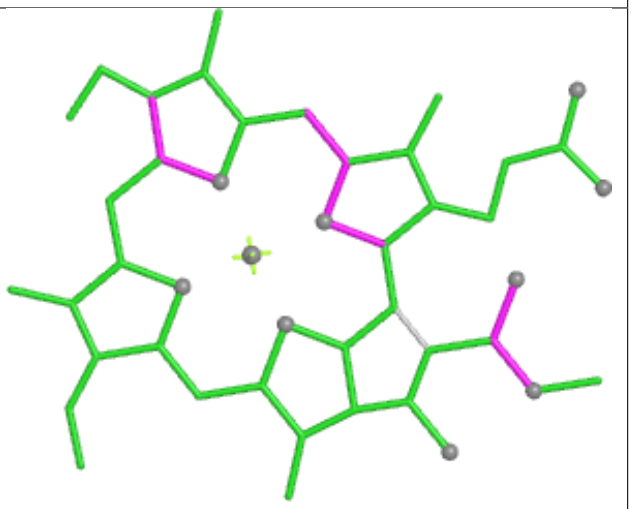

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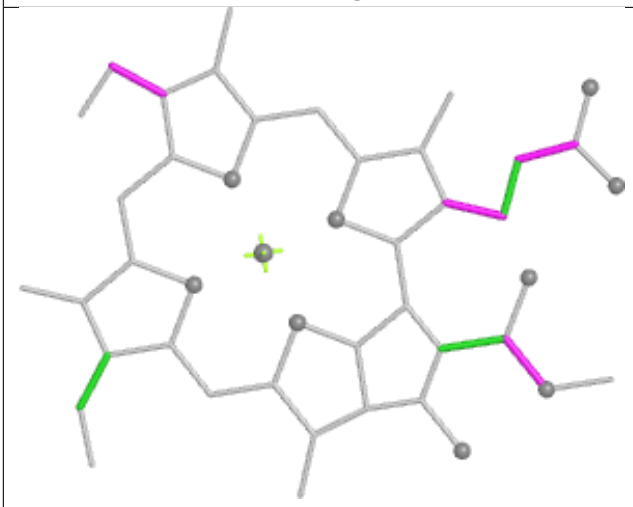

Torsions

Rings

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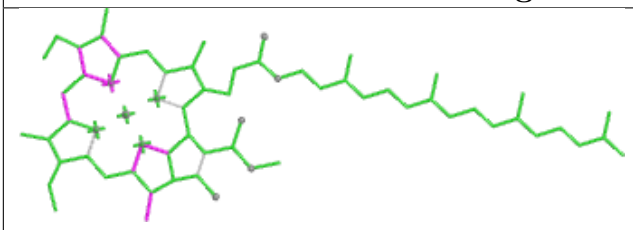

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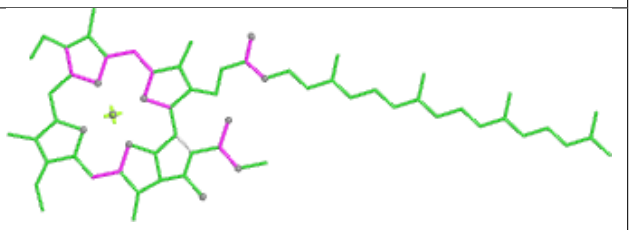

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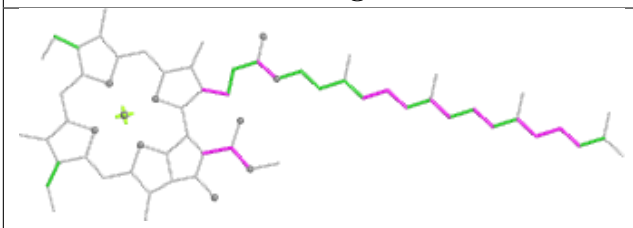

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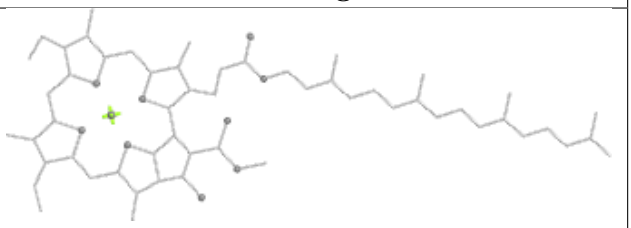

Rings

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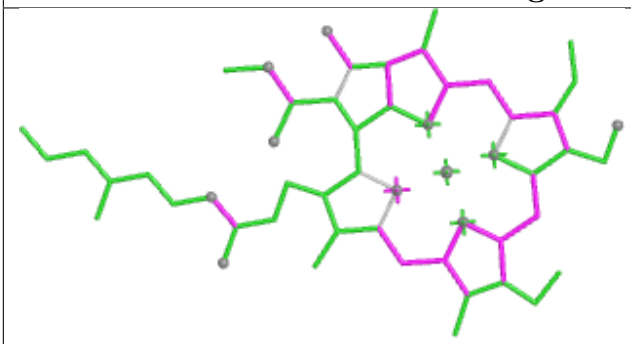

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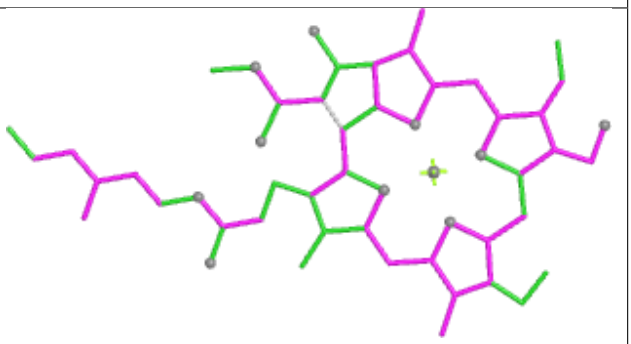

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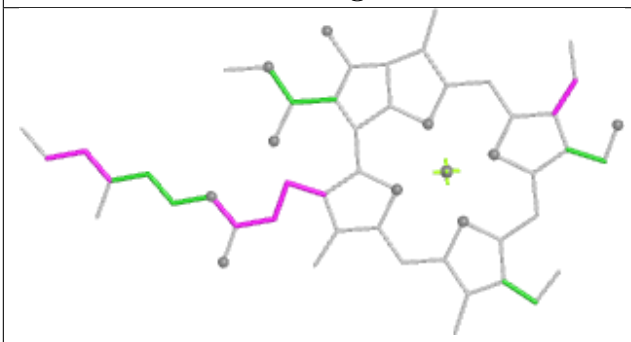

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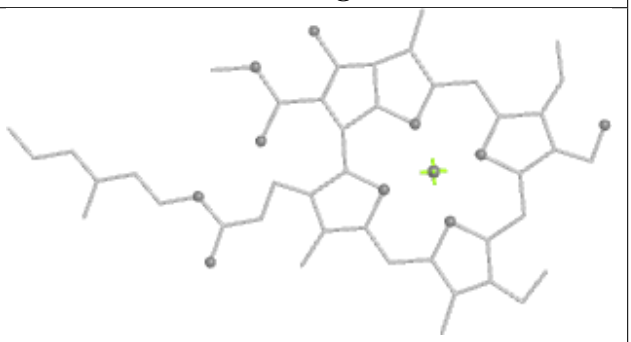

Rings

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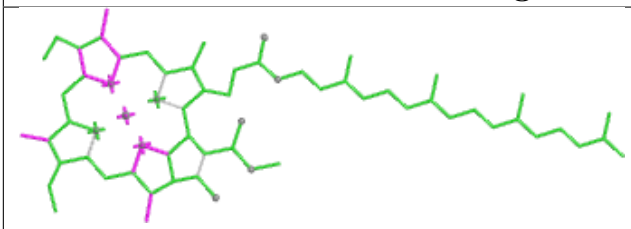

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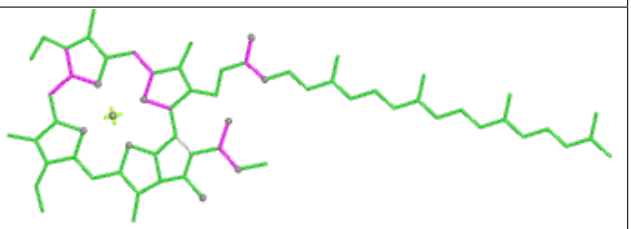

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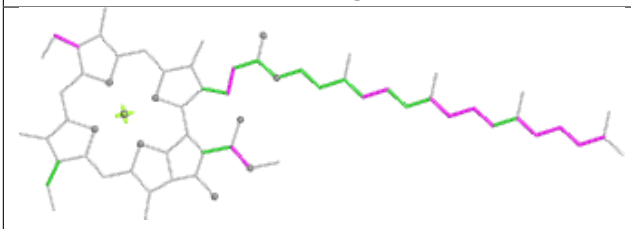

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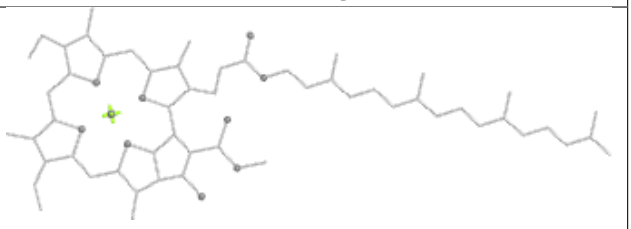

Rings

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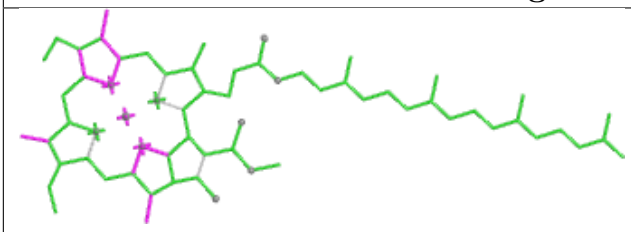
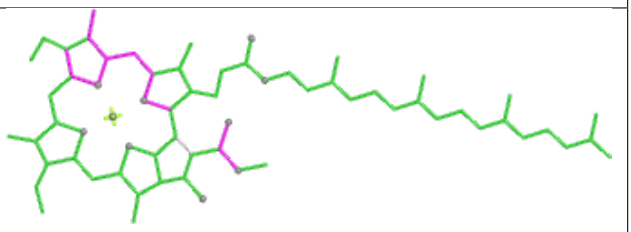
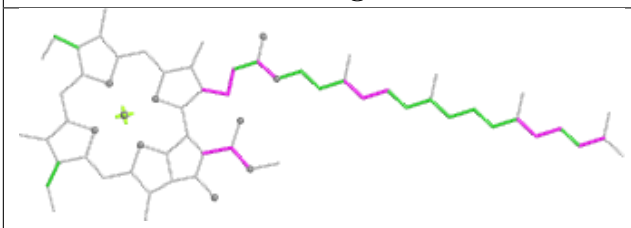
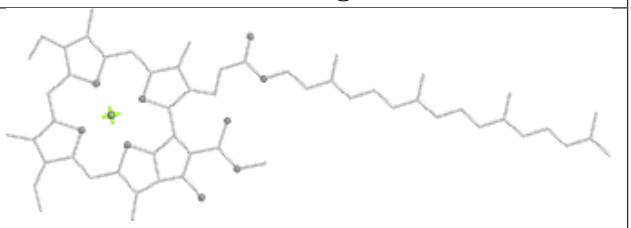
 Bond lengths	 Bond angles
 Torsions	 Rings

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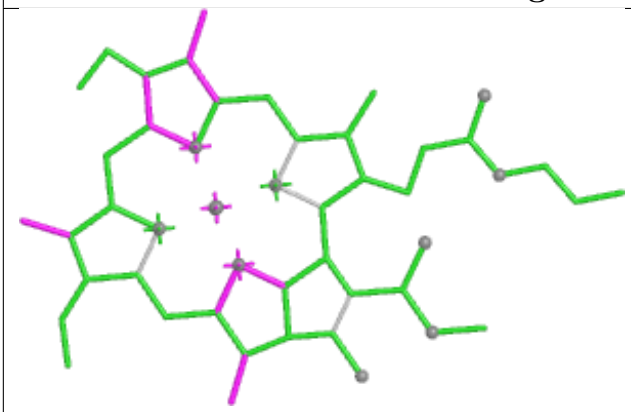
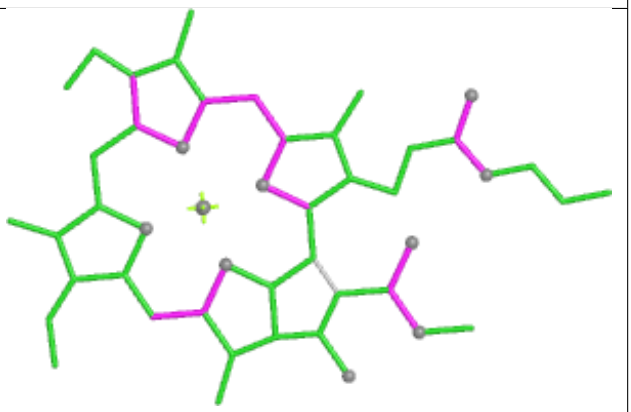
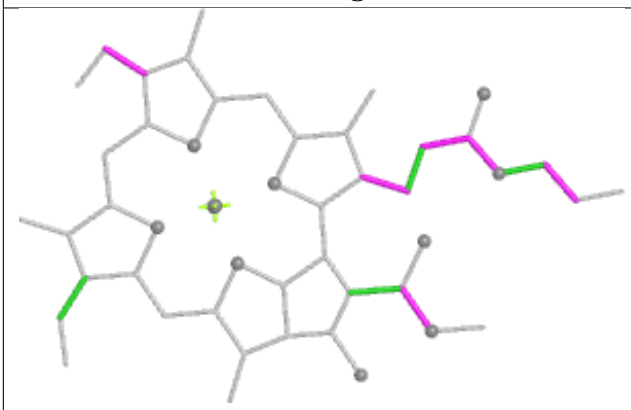
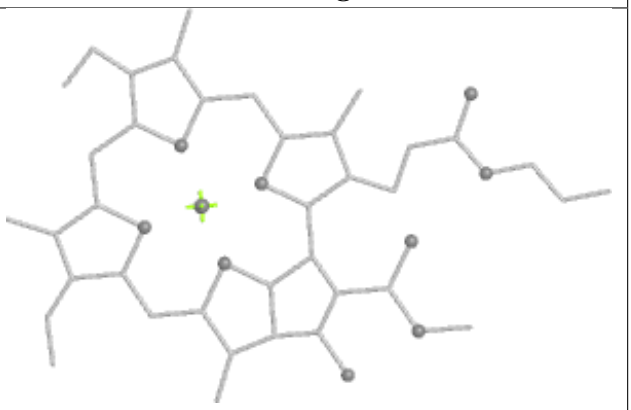
 Bond lengths	 Bond angles
 Torsions	 Rings

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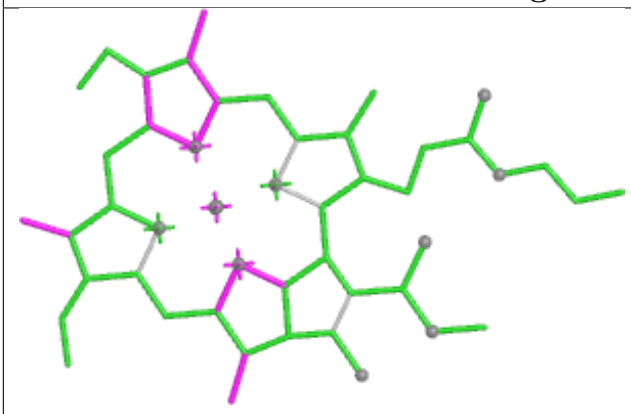
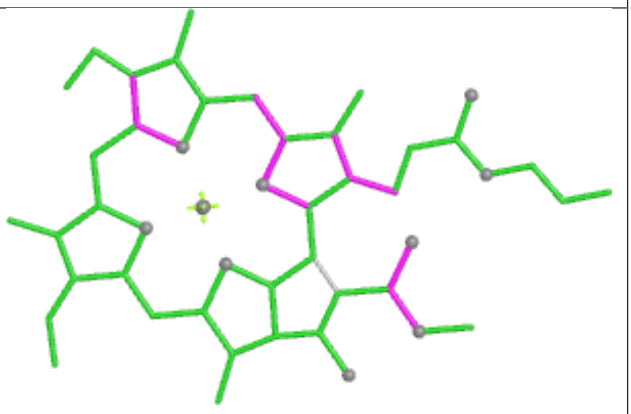
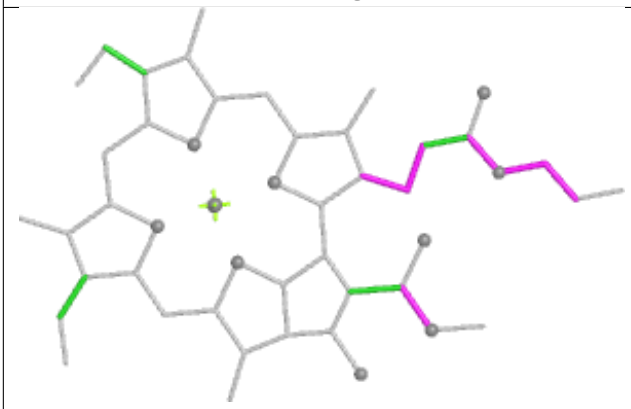
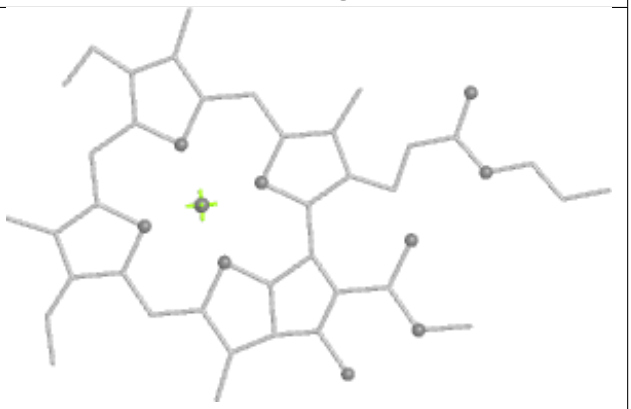
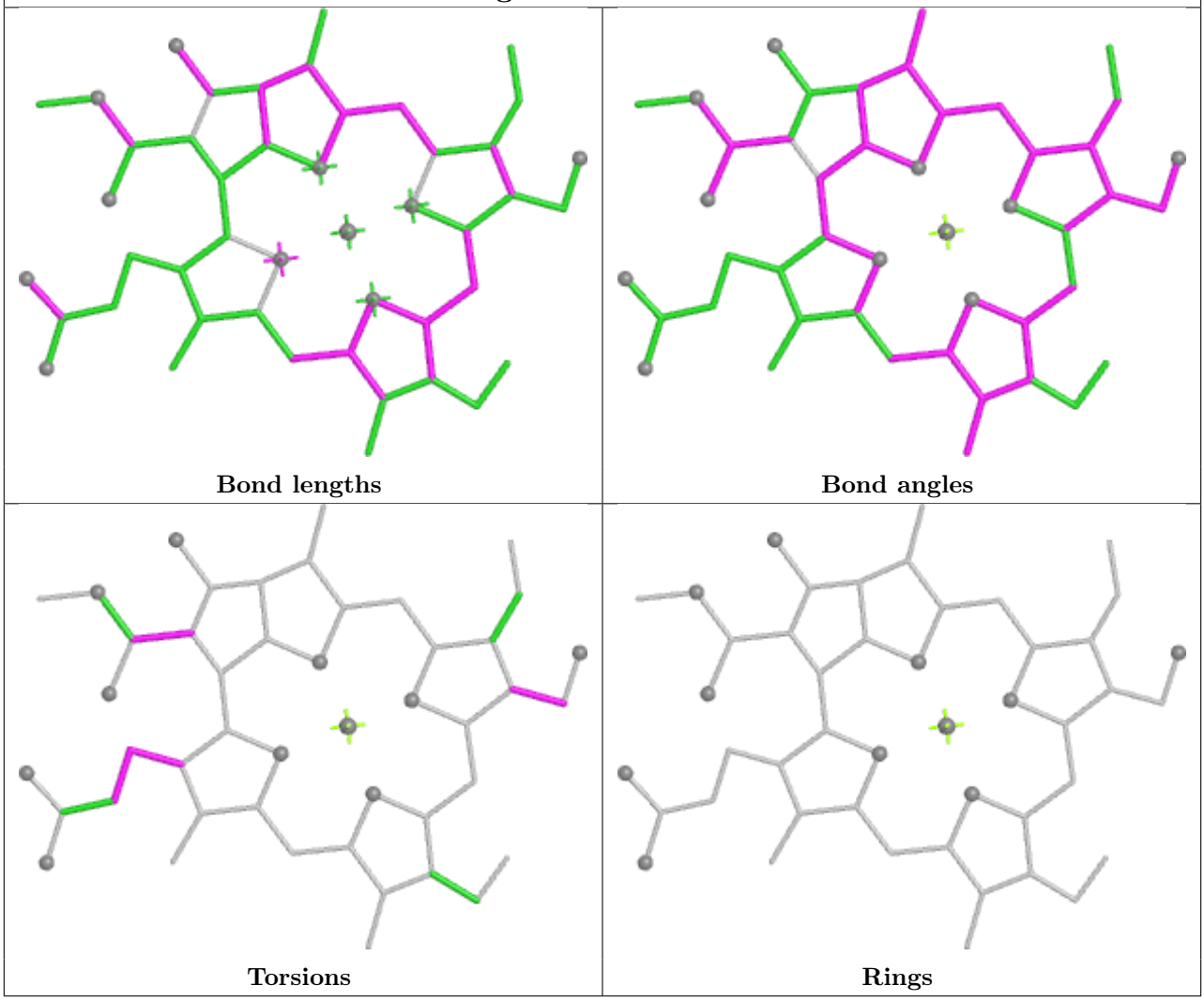
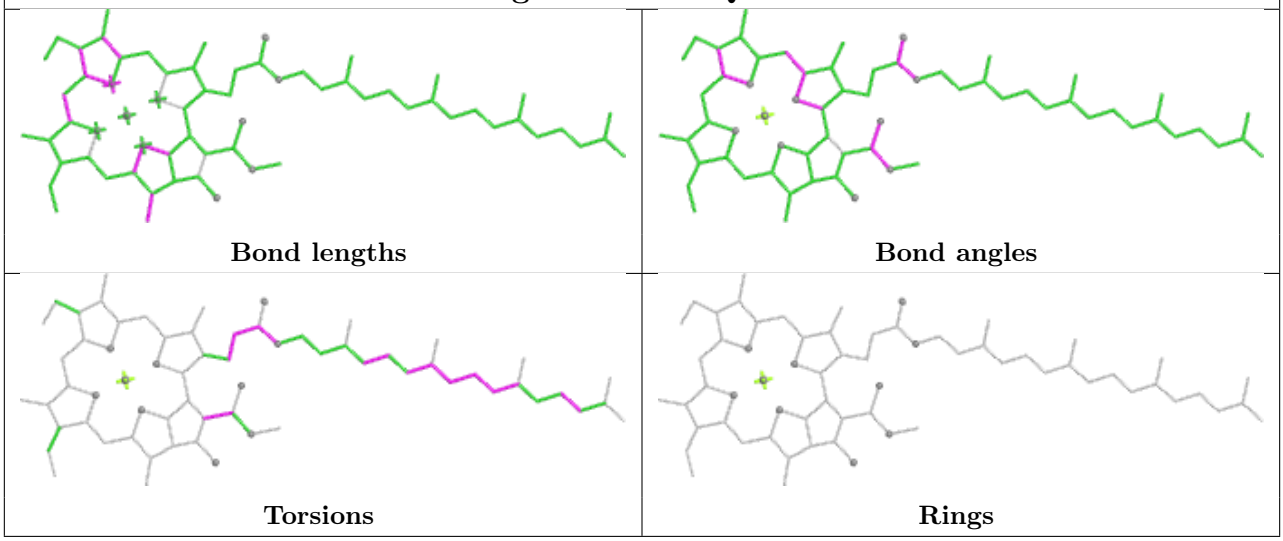
 Bond lengths	 Bond angles
 Torsions	 Rings

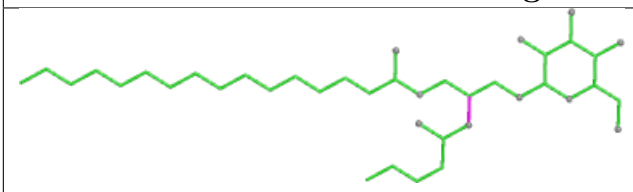
Ligand CHL 6 608



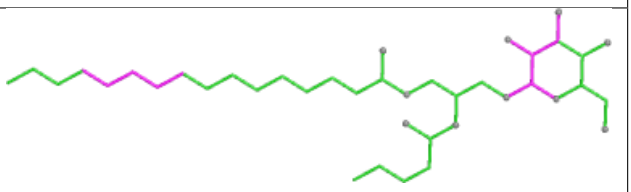
Ligand CLA BQ 602



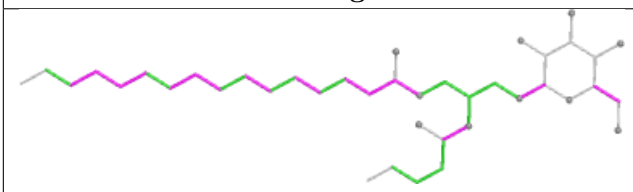
Ligand LMG v 623



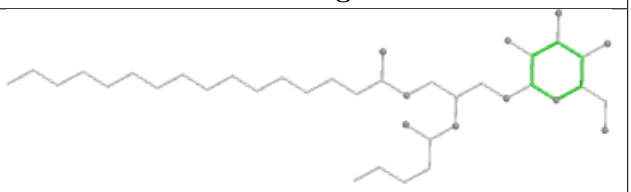
Bond lengths



Bond angles

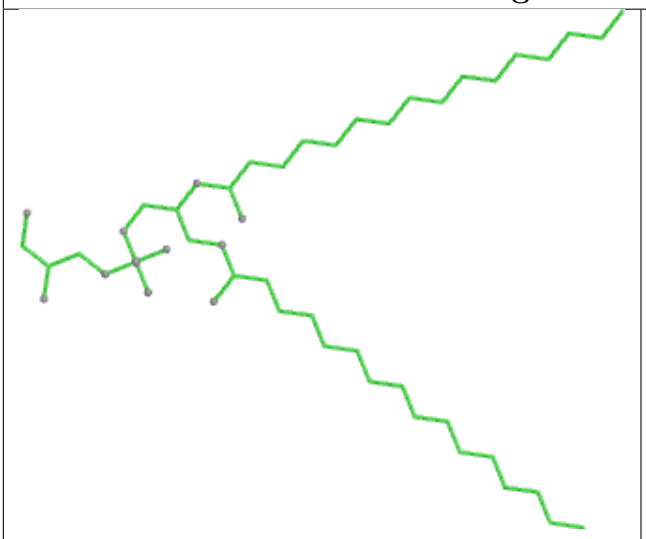


Torsions

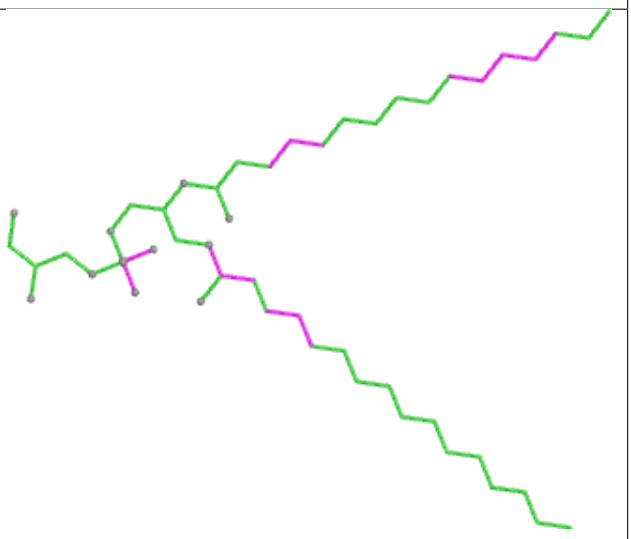


Rings

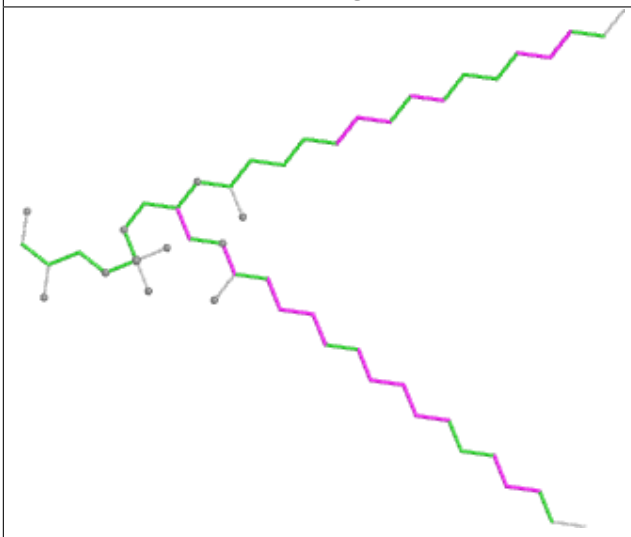
Ligand LHG Au 618



Bond lengths



Bond angles



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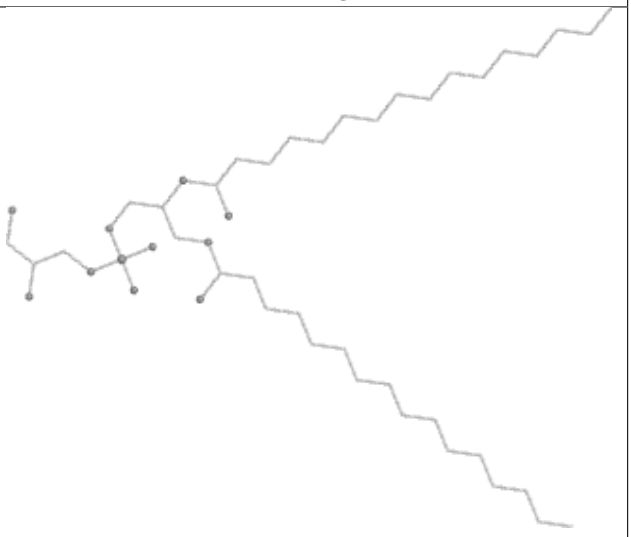
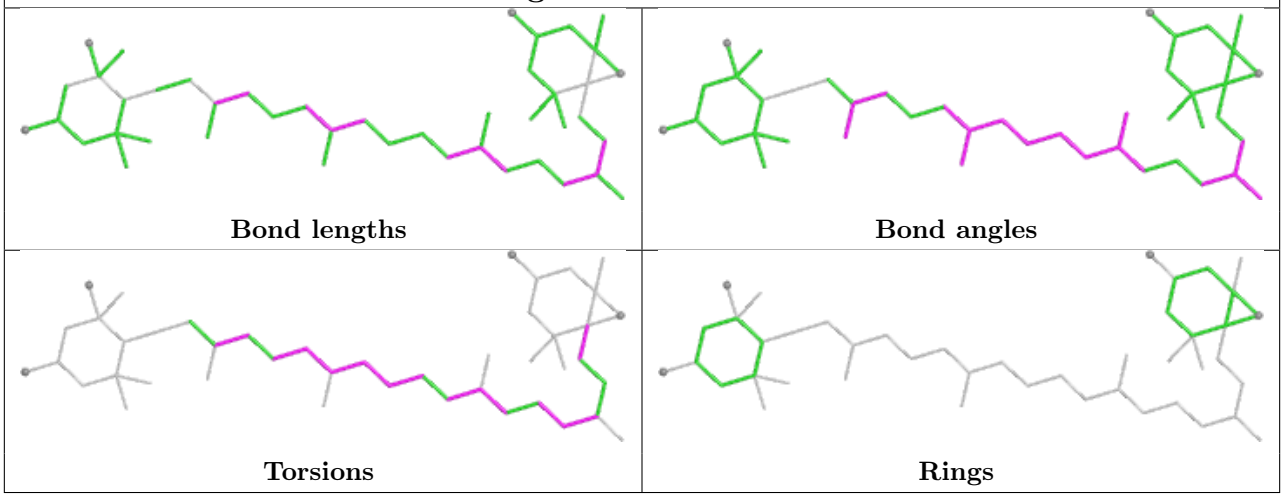


Rings

Ligand NEX 5 617



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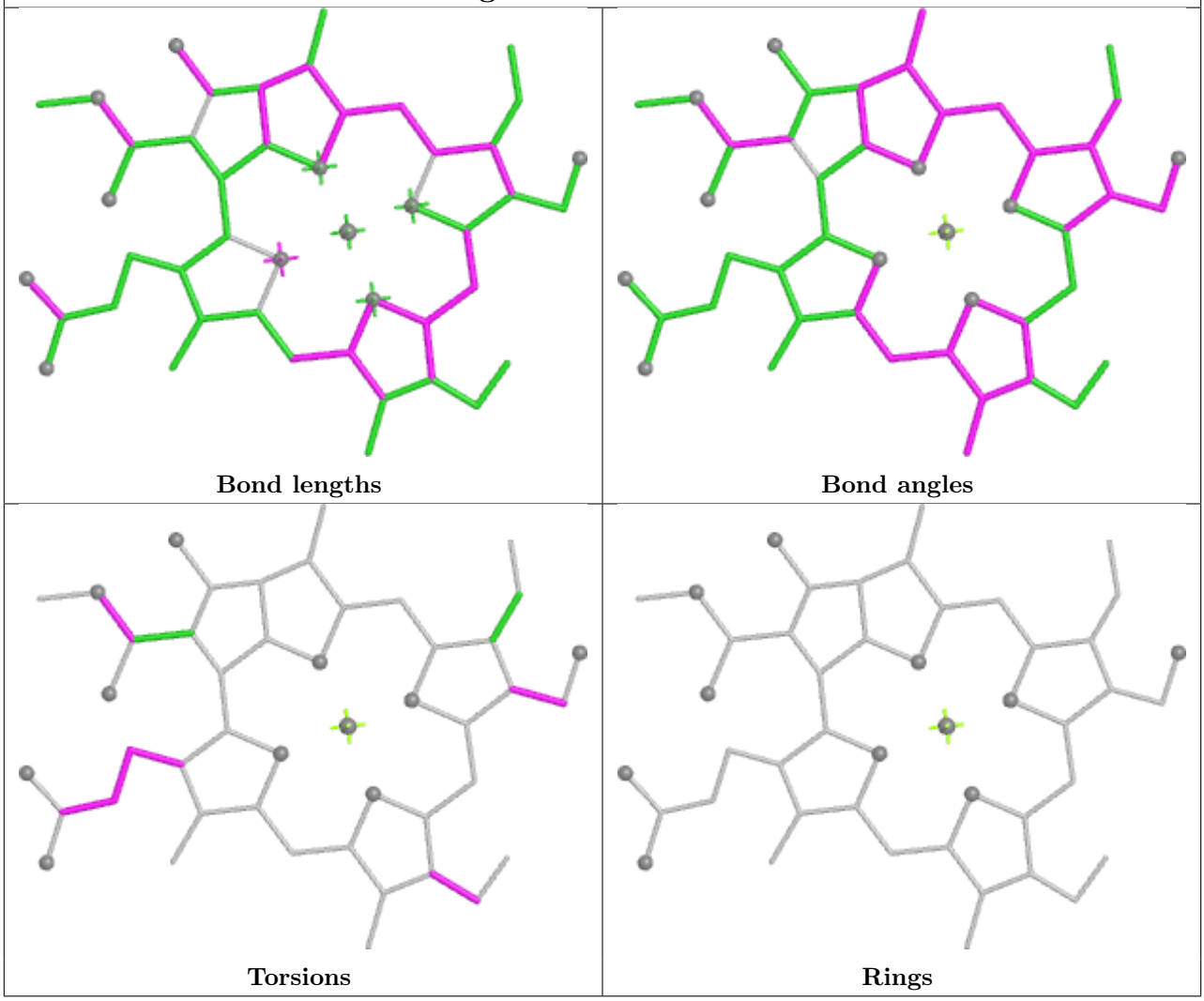

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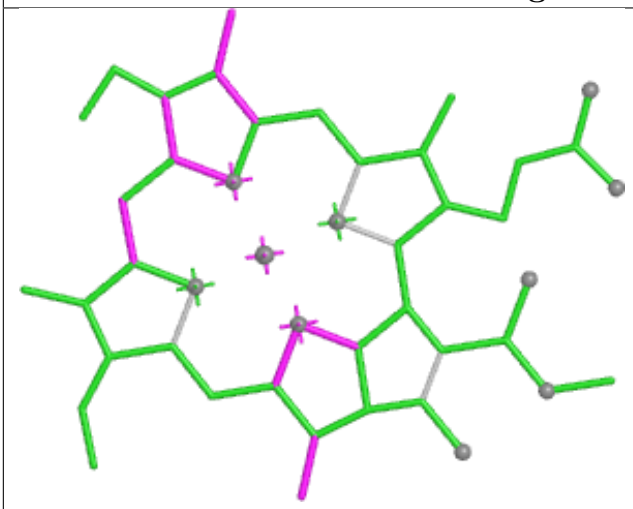

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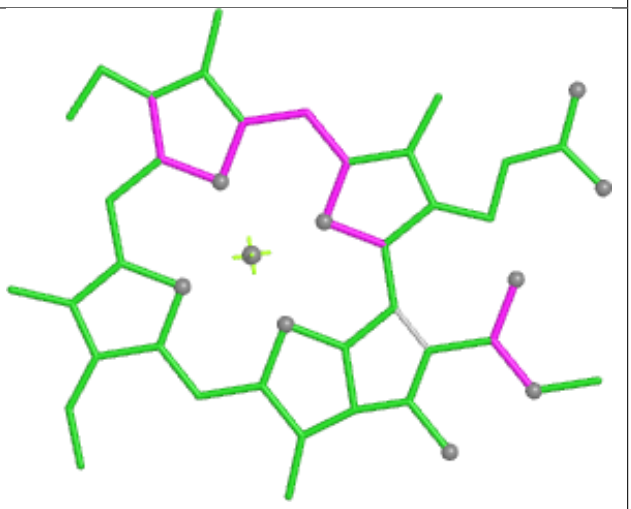

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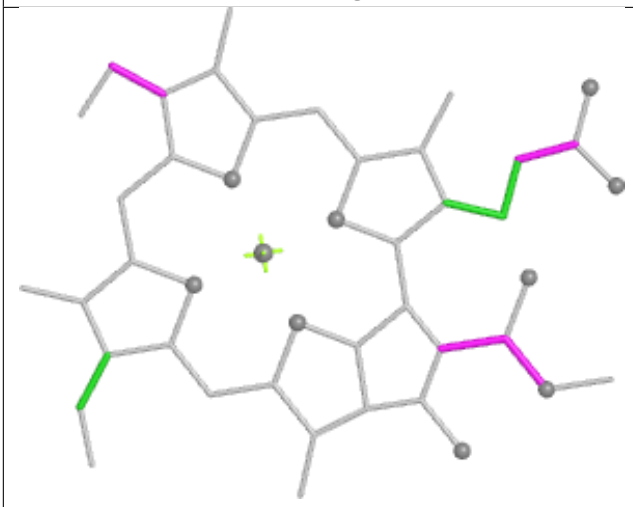

Torsions

Rings

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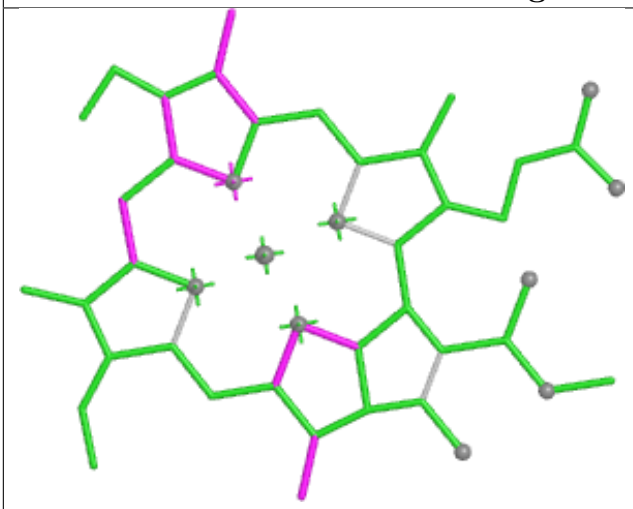

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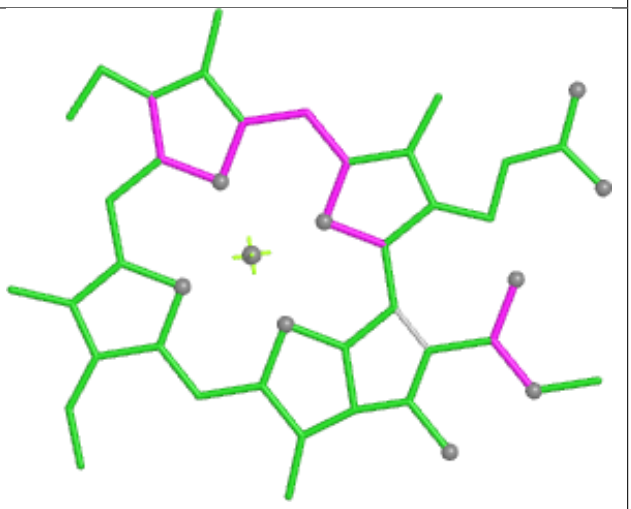

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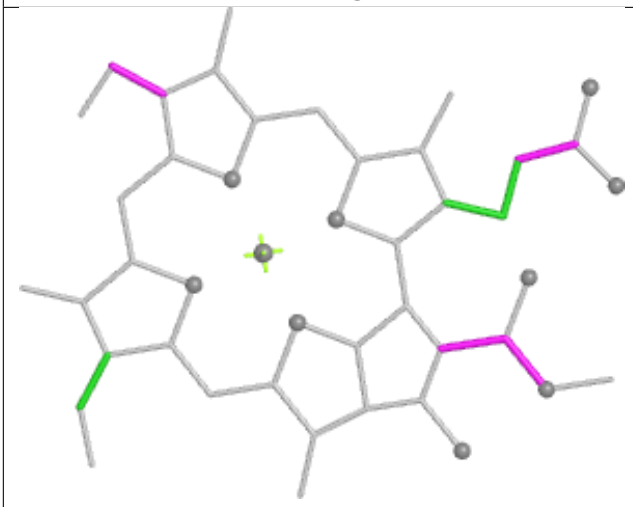
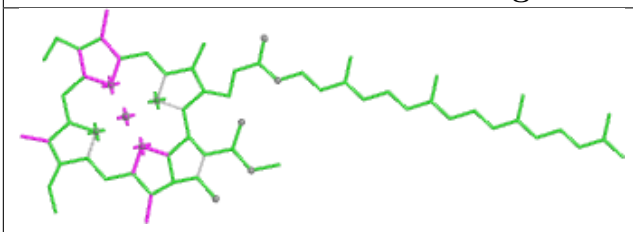


Torsions

Rings

Ligand CLA Aw 102



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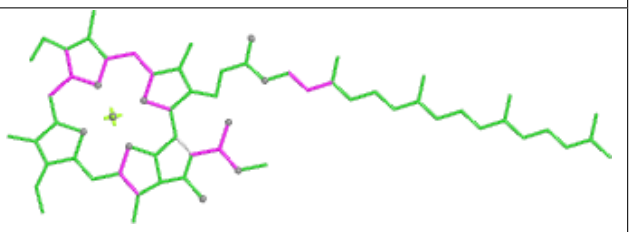
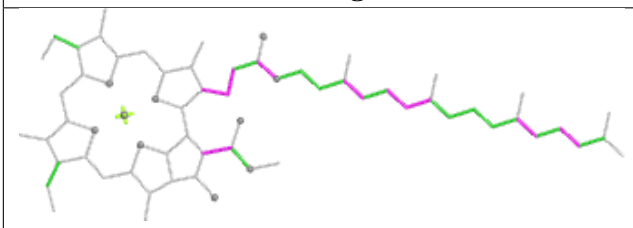


Bond angles



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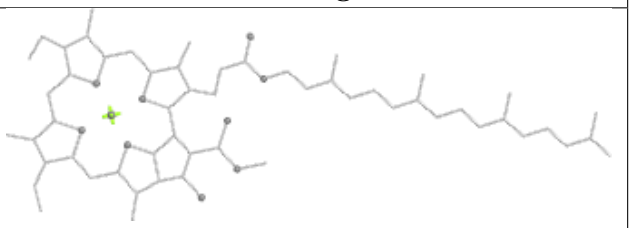
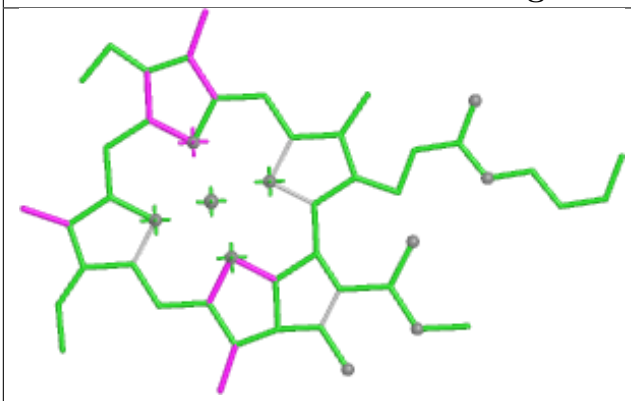
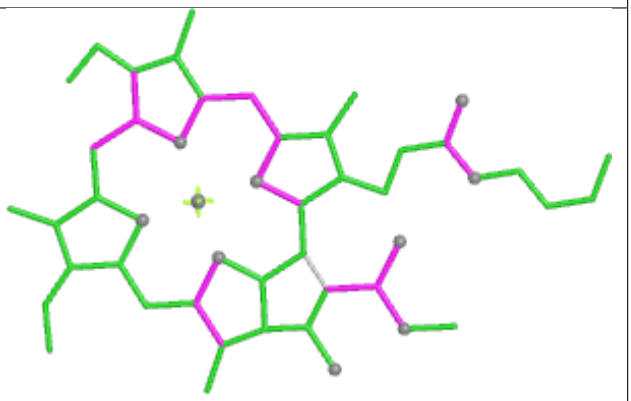
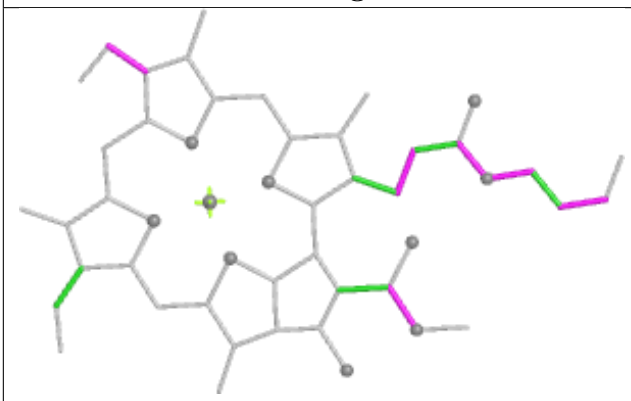
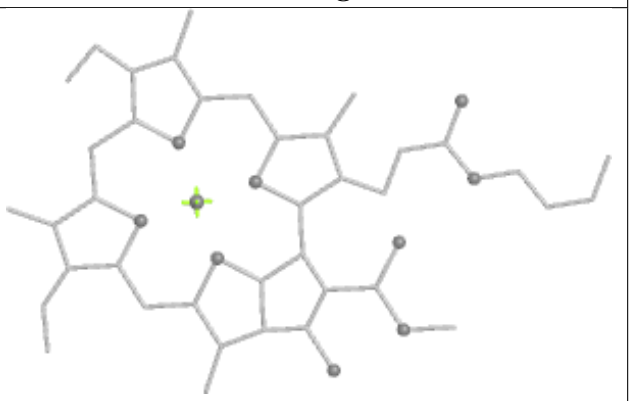


Rings

Ligand CLA S 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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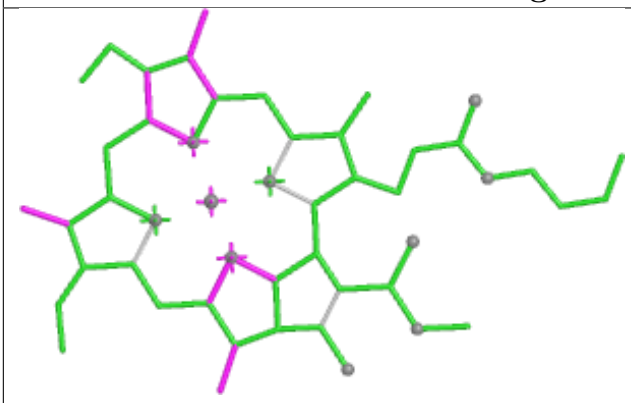
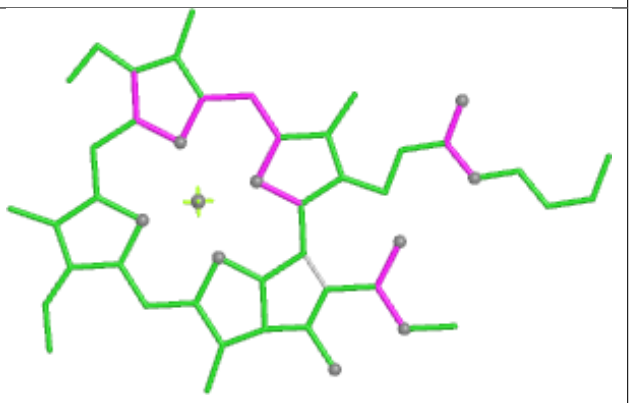
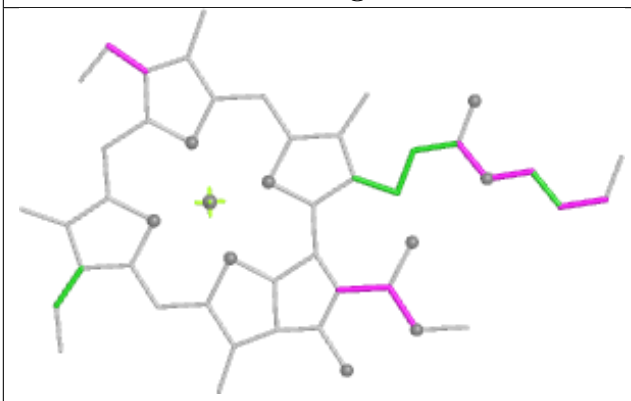
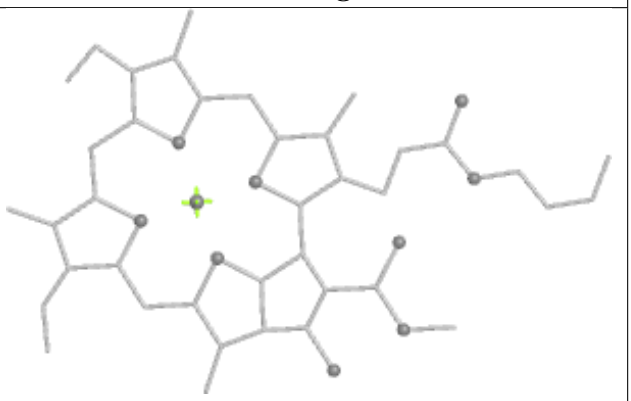
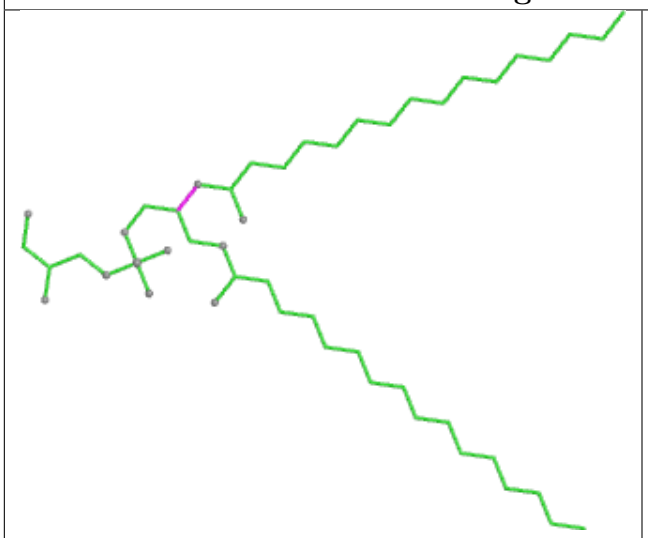
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A2 618



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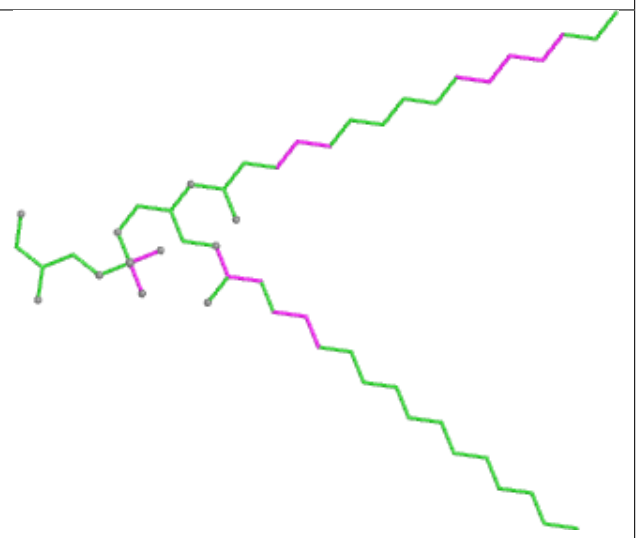
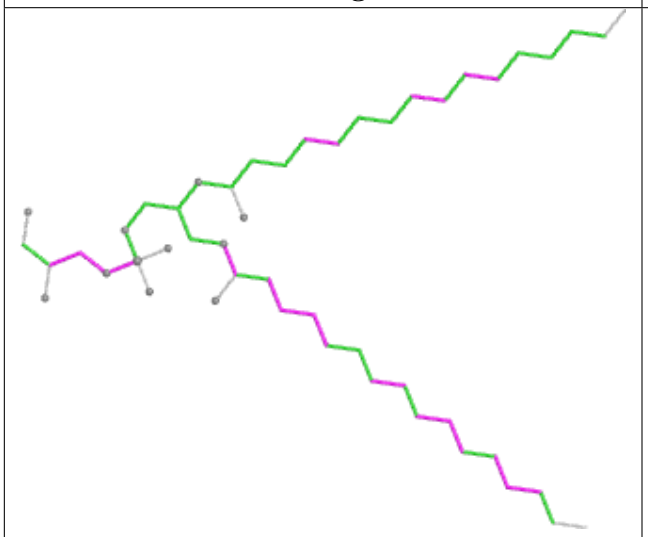


Bond angles



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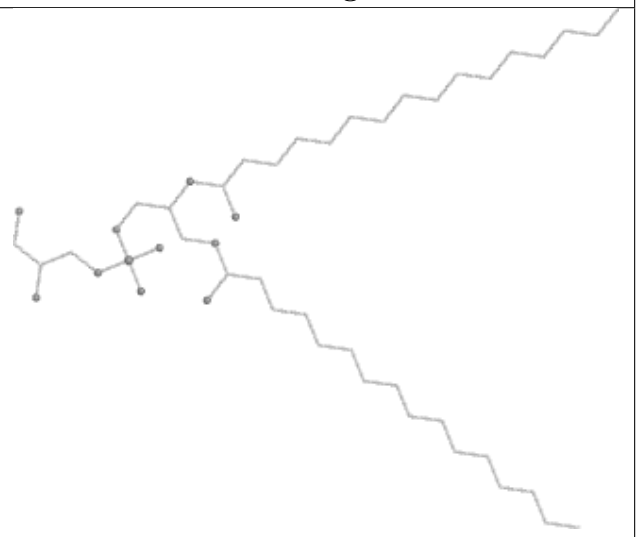
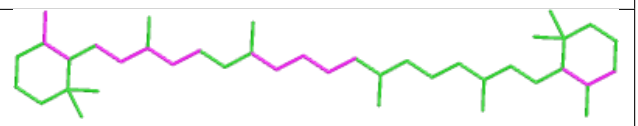


Rings

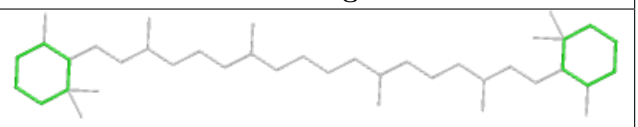
Ligand BCR c 515

Bond lengths



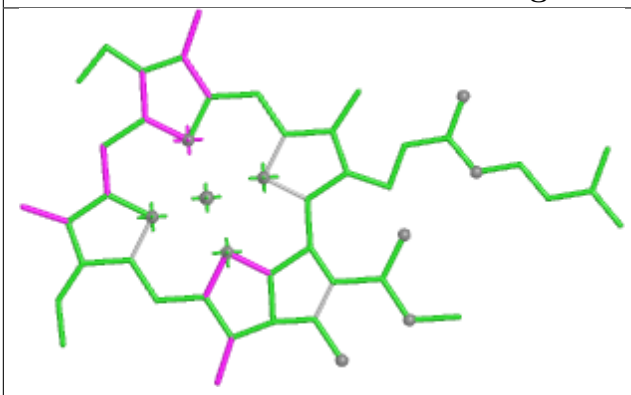
Bond angles

Torsions

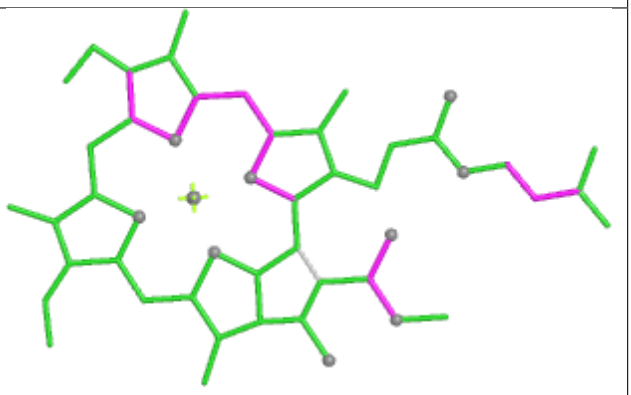


Rings

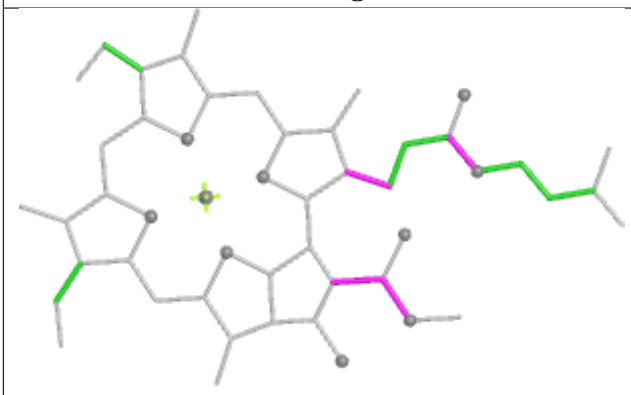
Ligand CLA s 604



Bond lengths



Bond angles



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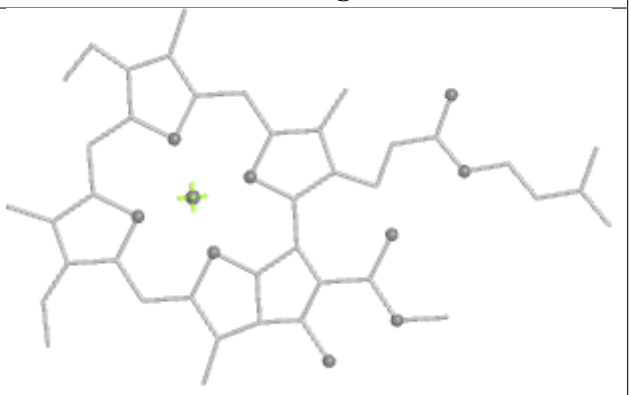
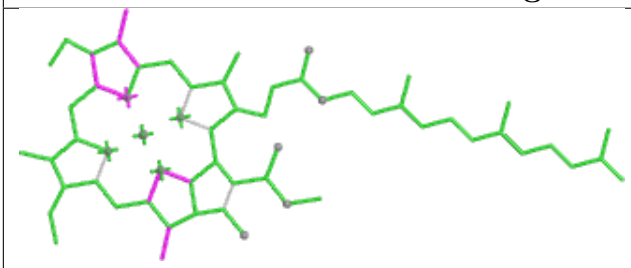


Rings

Ligand CLA A 410



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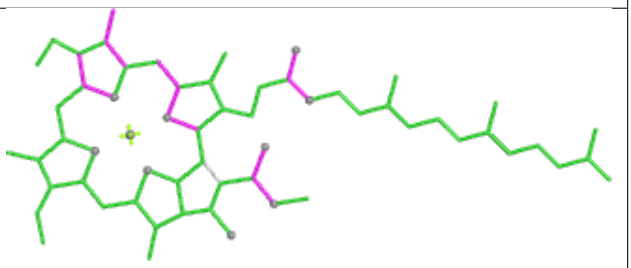
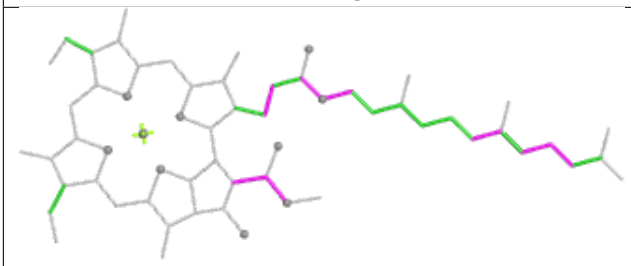


Bond angles



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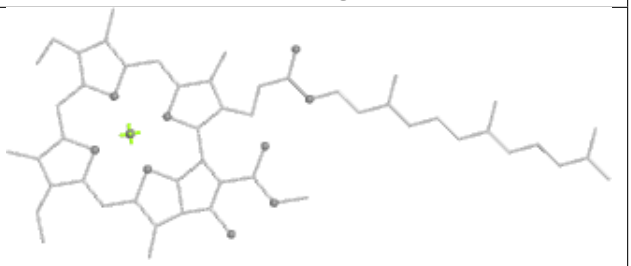
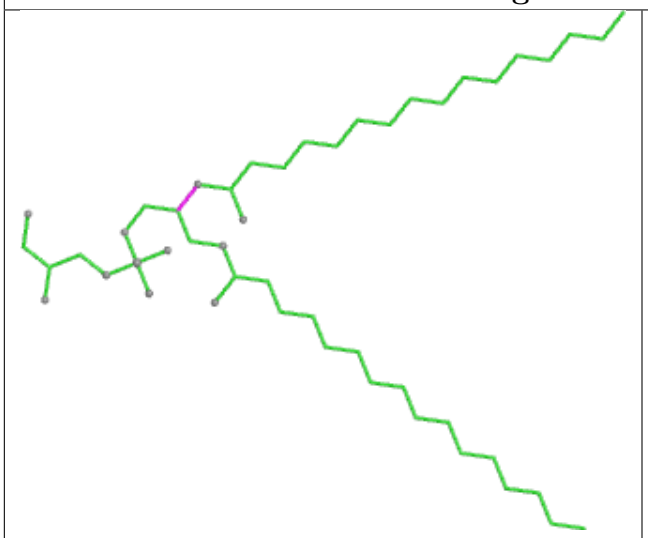
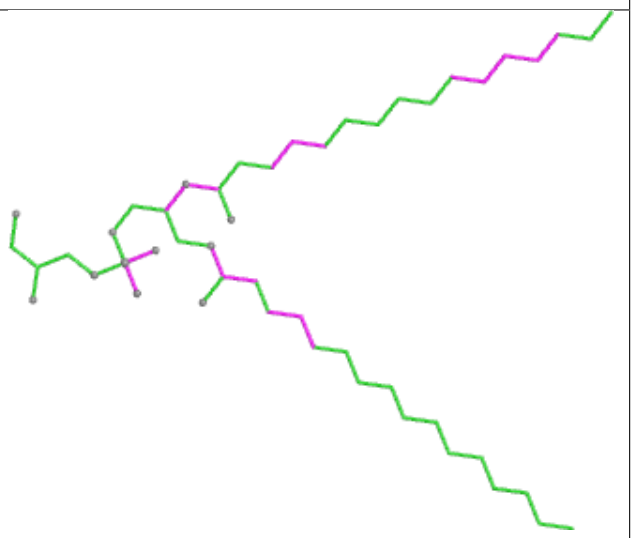


Rings

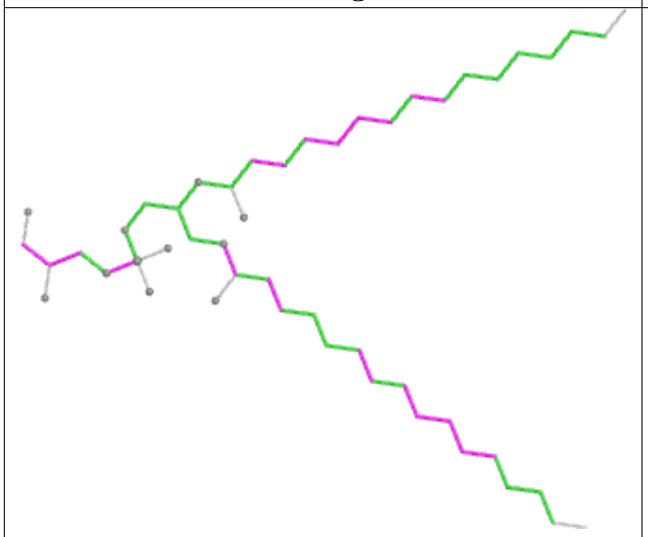
Ligand LHG BE 624



Bond lengths



Bond angles



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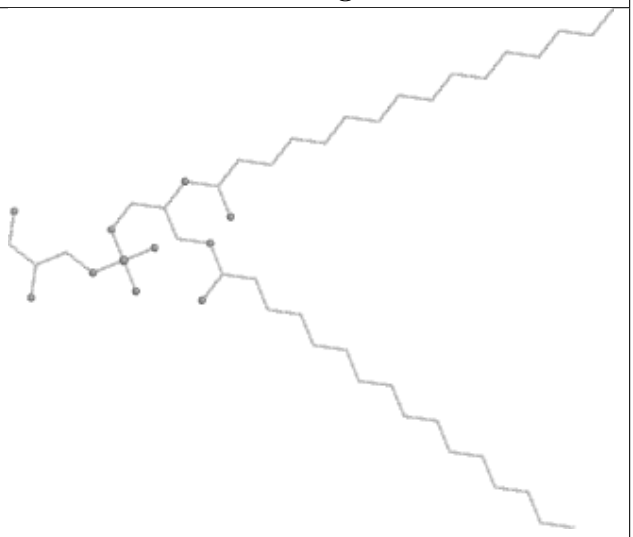
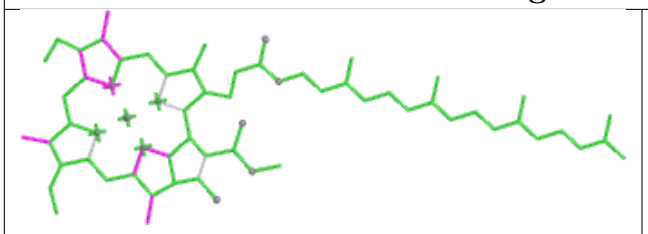


Rings

Ligand CLA v 614



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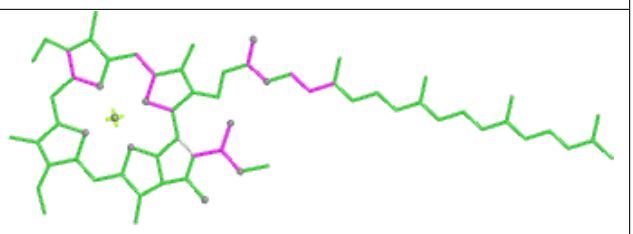
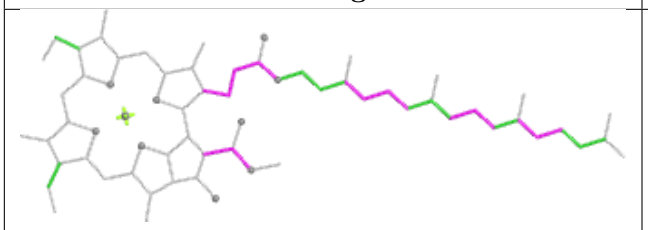


Bond angles



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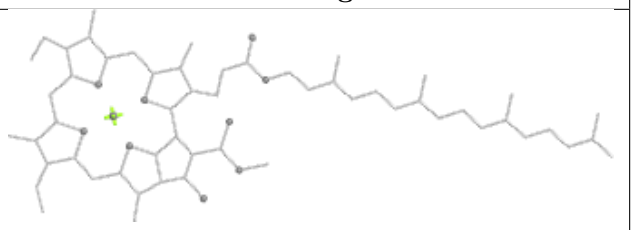
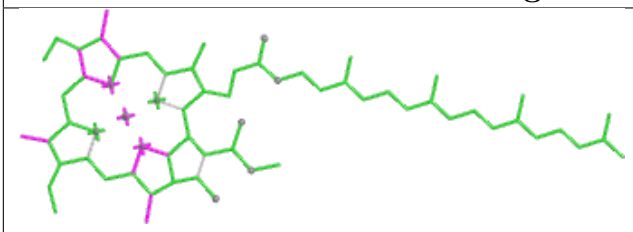
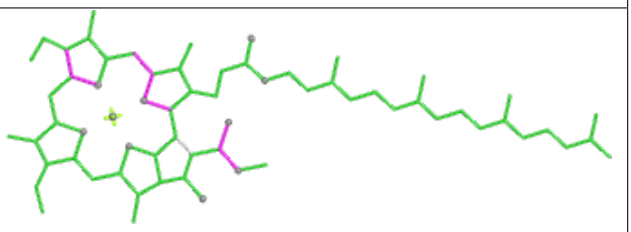


Rings

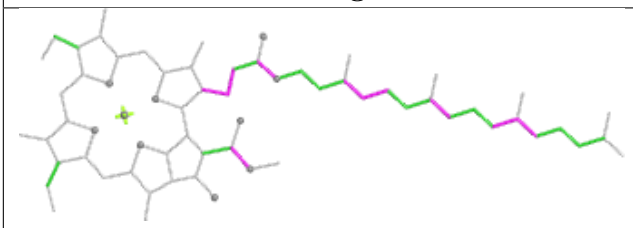
Ligand CLA Y 314



Bond lengths



Bond angles



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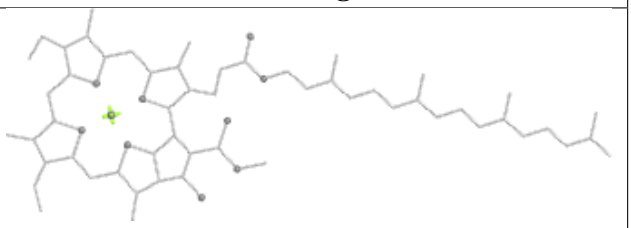
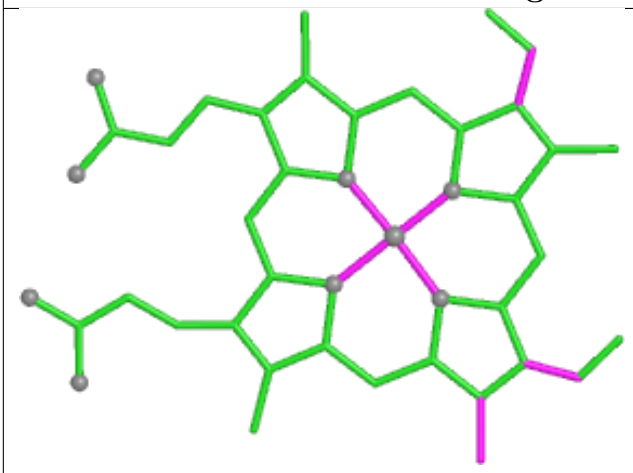
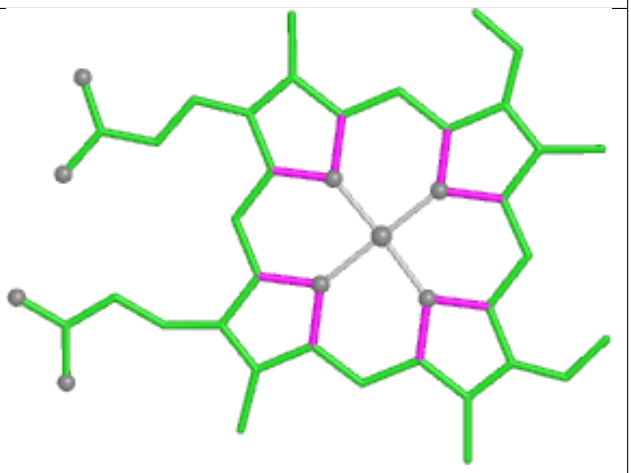


Rings

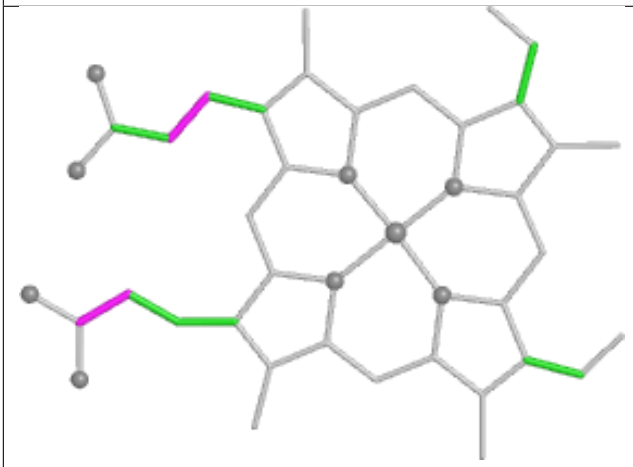
Ligand HEM f 102



Bond lengths



Bond angles



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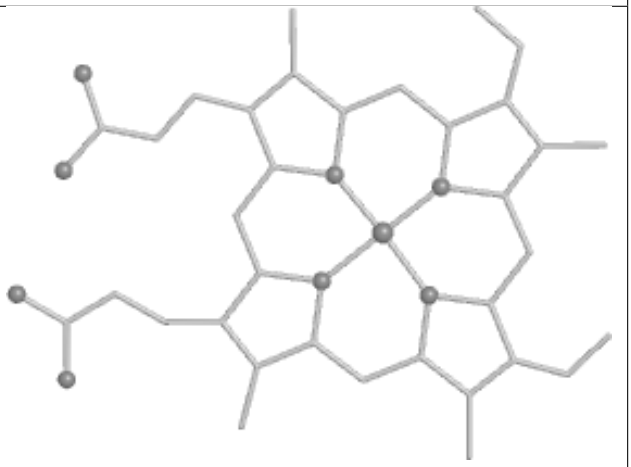
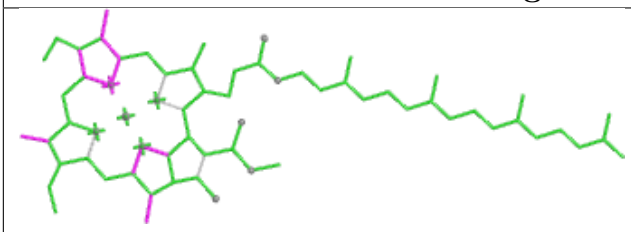
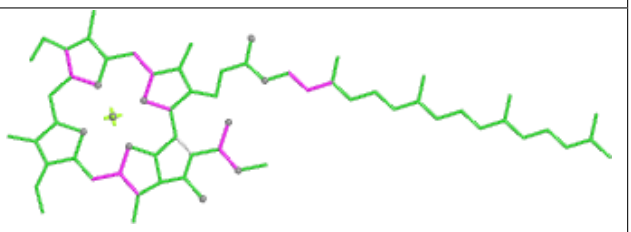


Rings

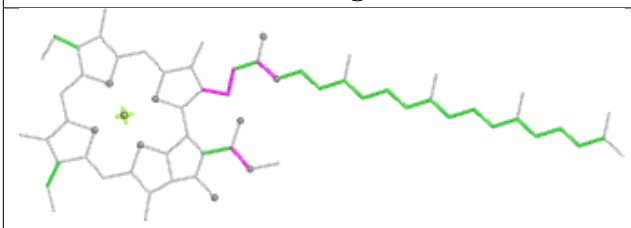
Ligand CLA A 406



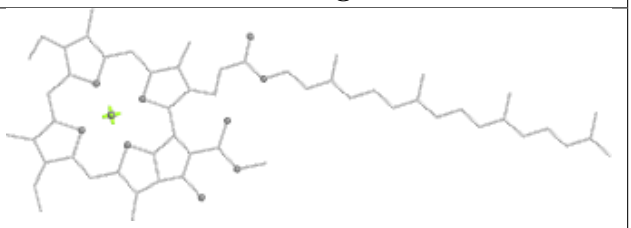
Bond lengths



Bond angles

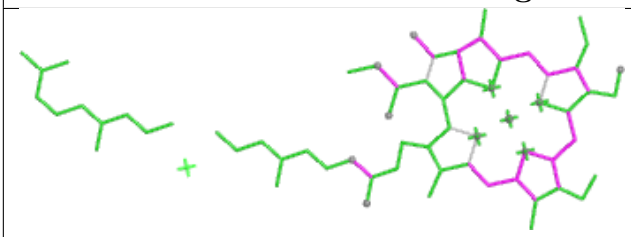


Torsions

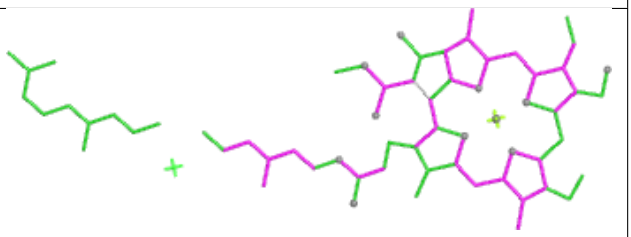


Rings

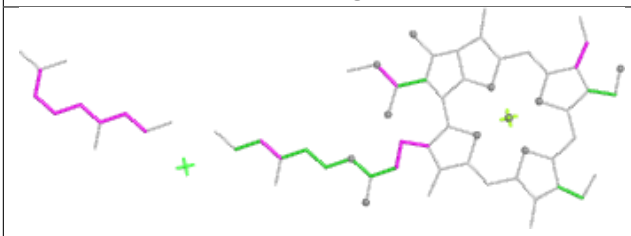
Ligand CHL BJ 607



Bond lengths



Bond angles



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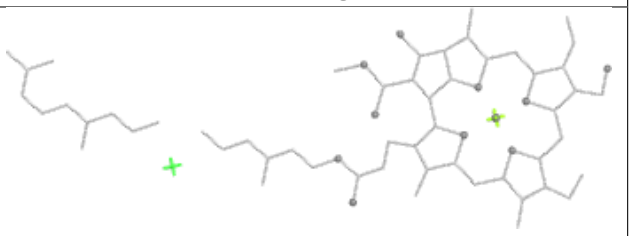
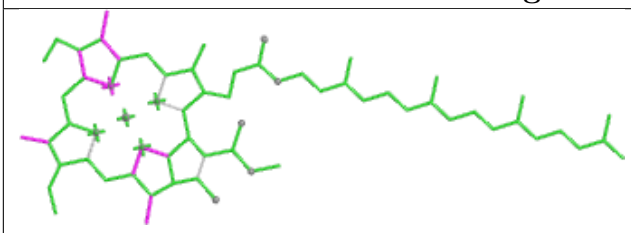
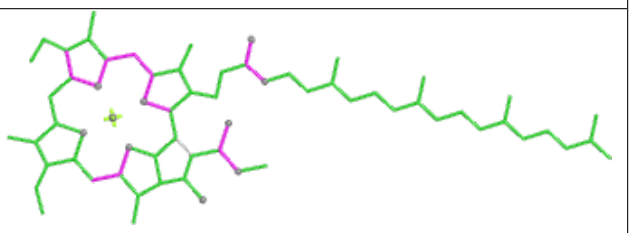


Rings

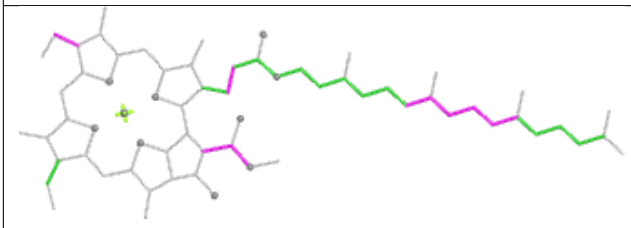
Ligand CLA N 602



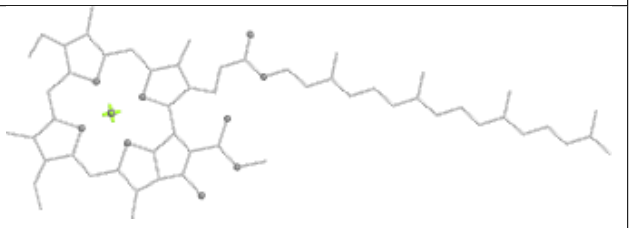
Bond lengths



Bond angles

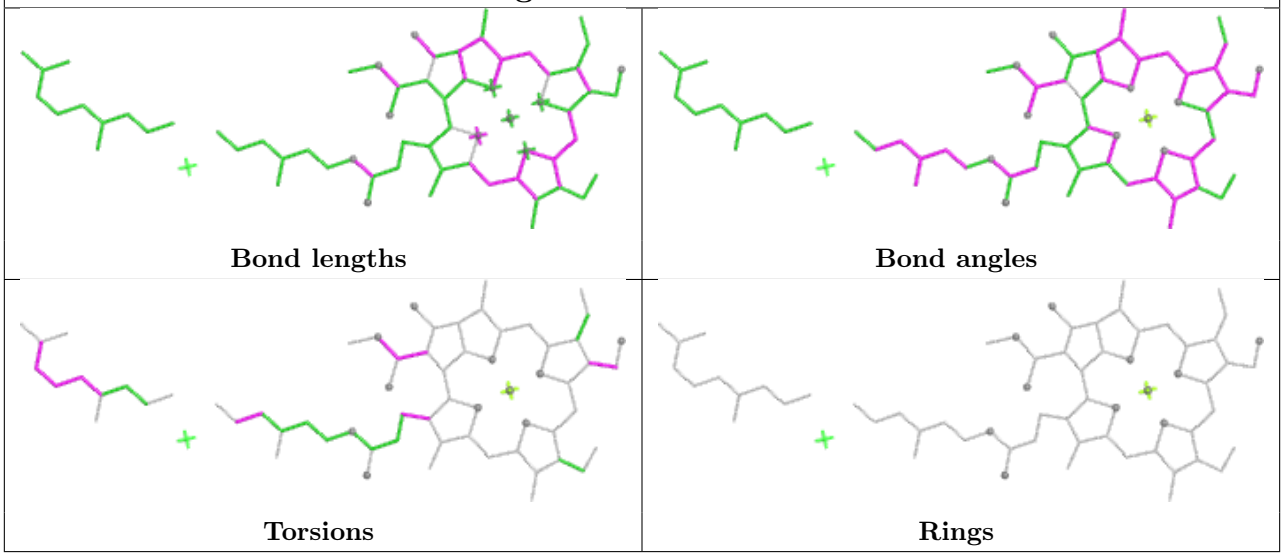


Torsions

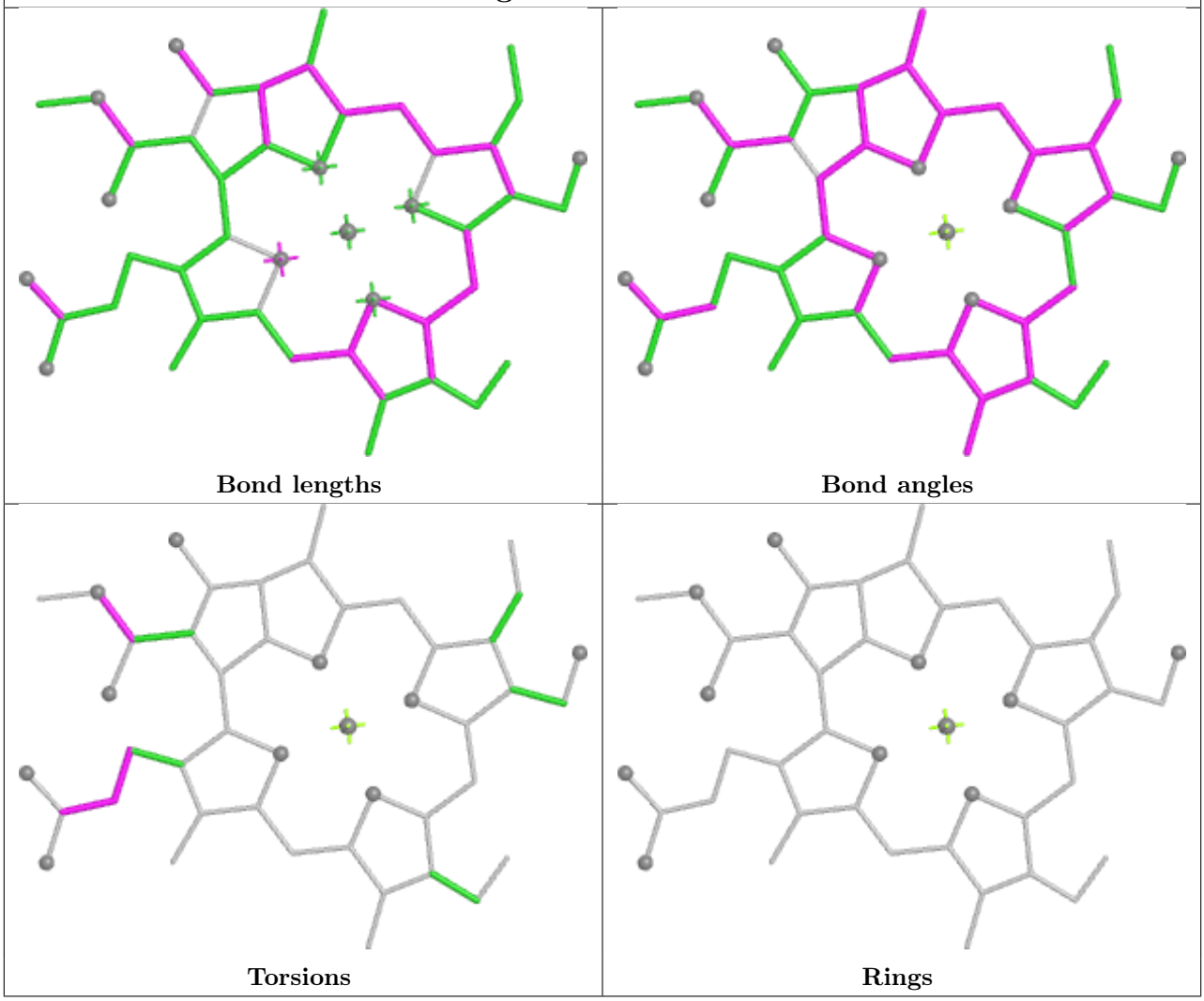


Rings

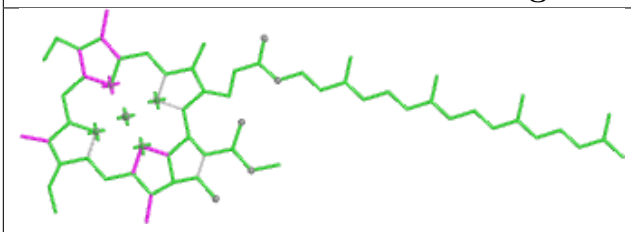
Ligand CHL A2 608



Ligand CHL 7 306



Ligand CLA c 506



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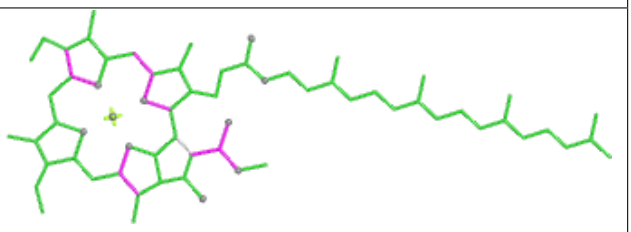
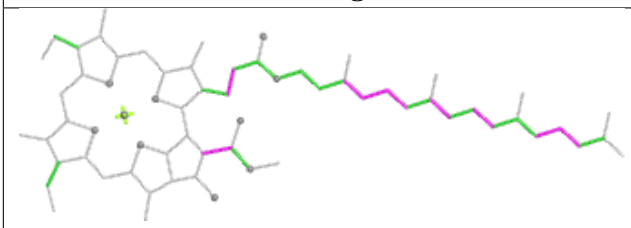


Bond angles



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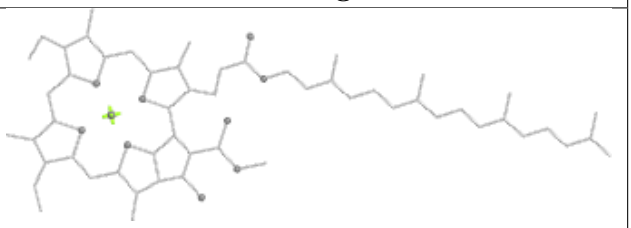
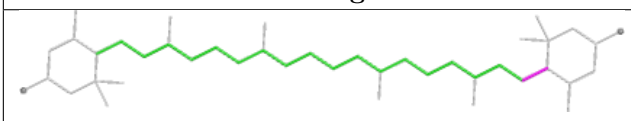


Rings

Ligand LUT BV 615

Bond lengths

Bond angles



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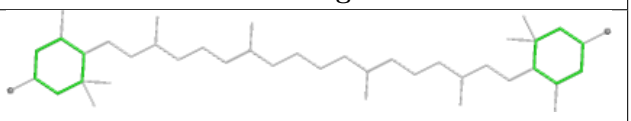
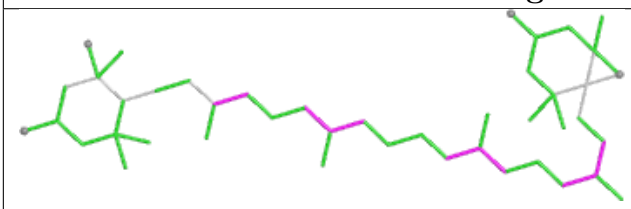


Rings

Ligand NEX 9 617



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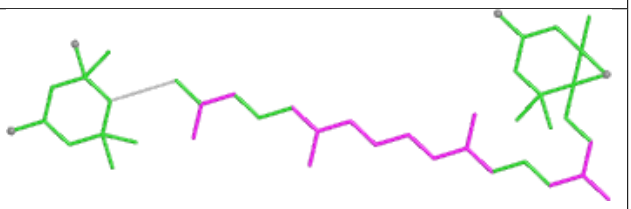
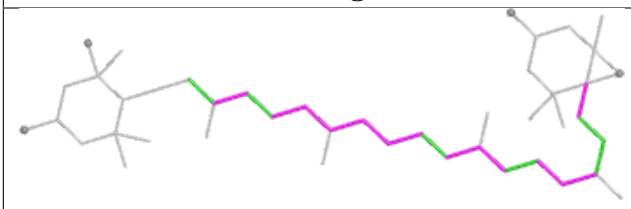


Bond angles



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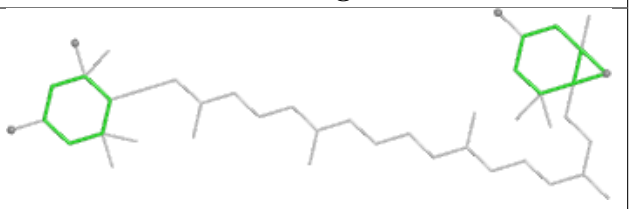
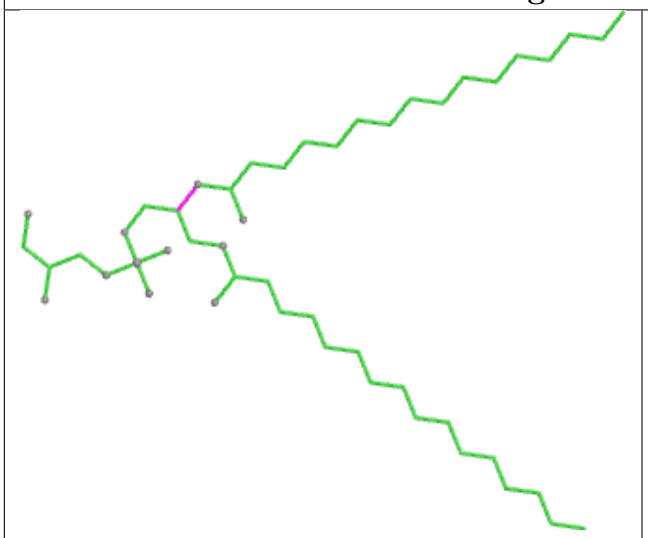
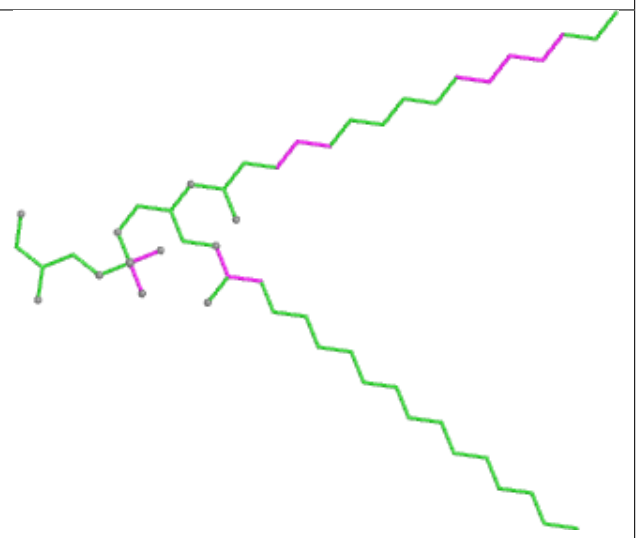


Rings

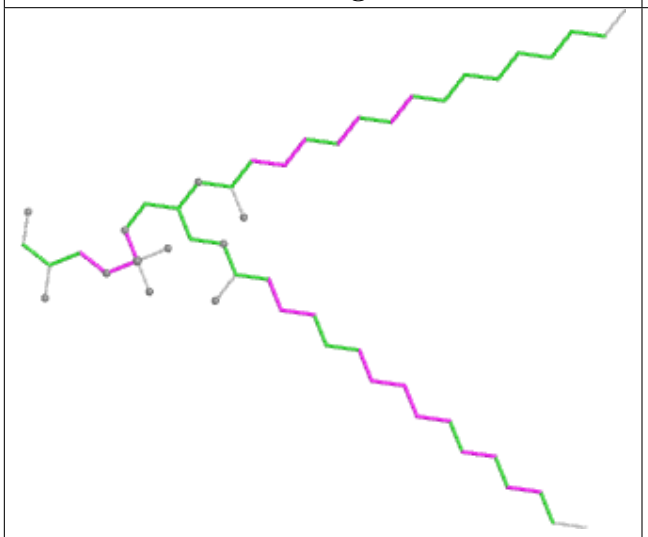
Ligand LHG 2 406



Bond lengths



Bond angles



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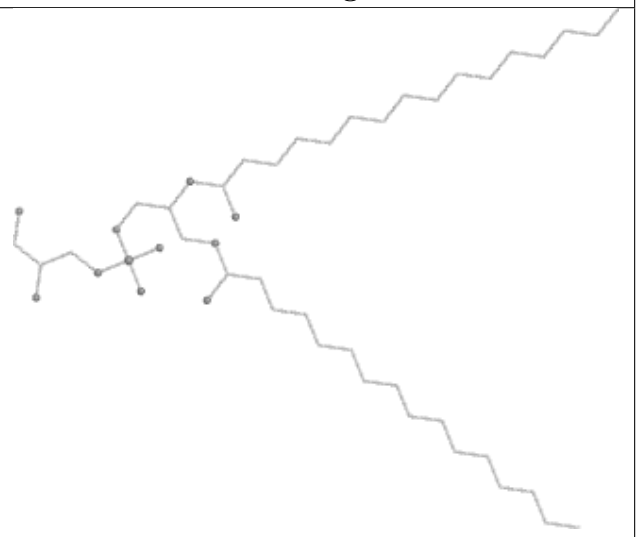
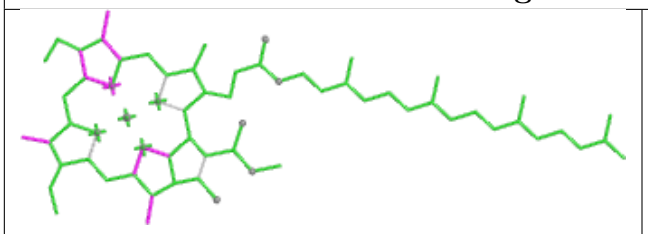


Rings

Ligand CLA BF 506



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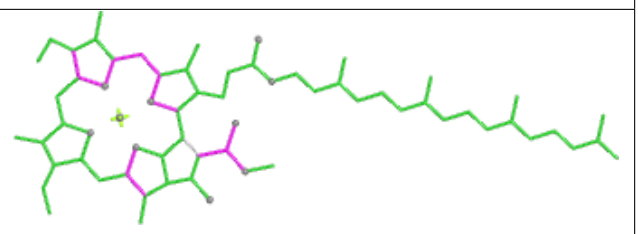
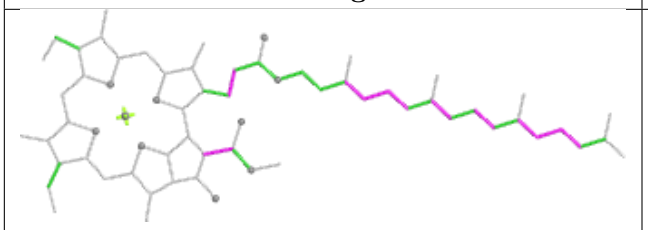


Bond angles



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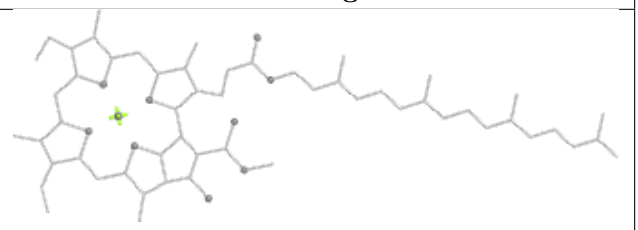
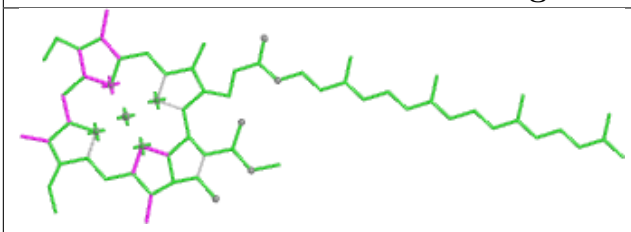
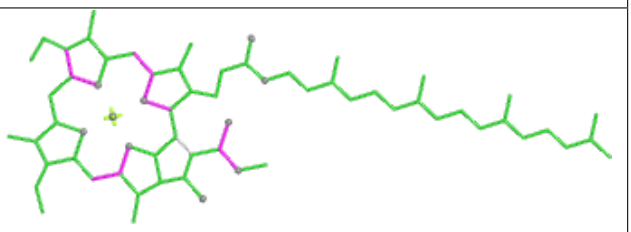
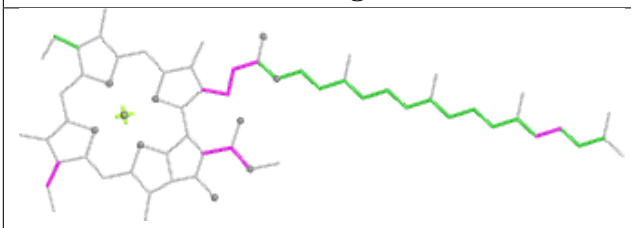
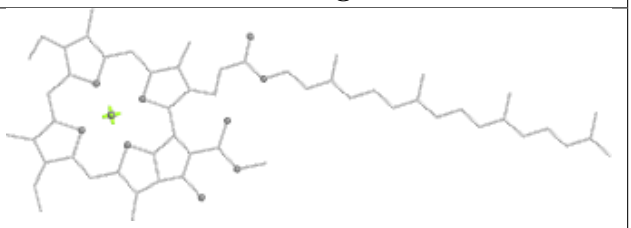
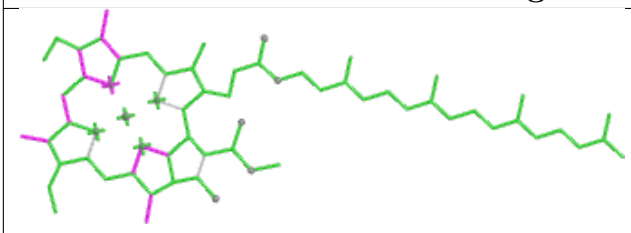
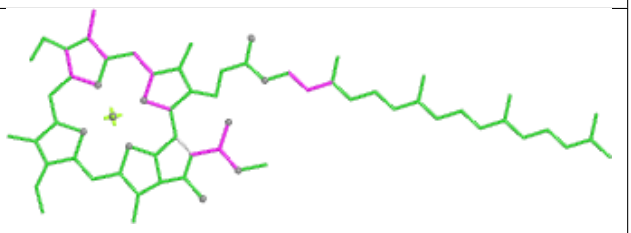
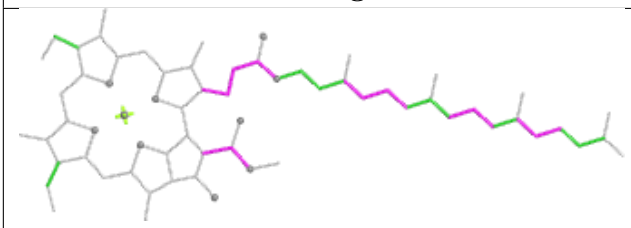
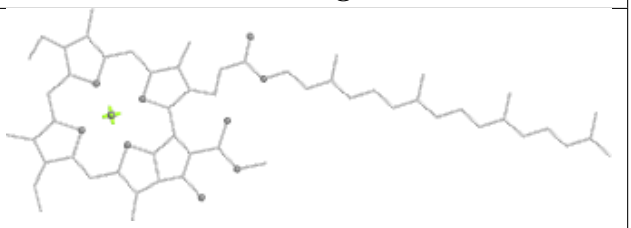
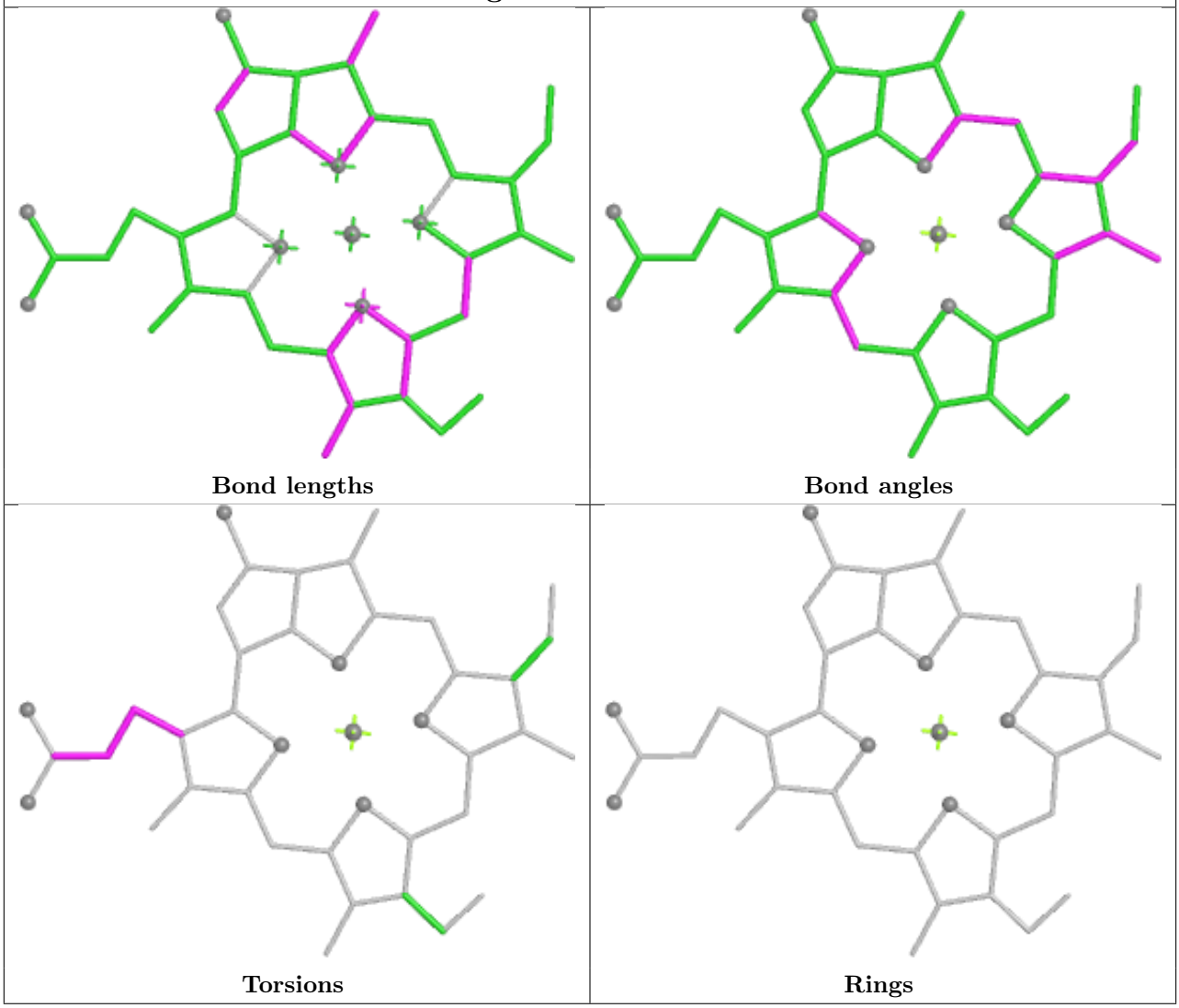


Rings

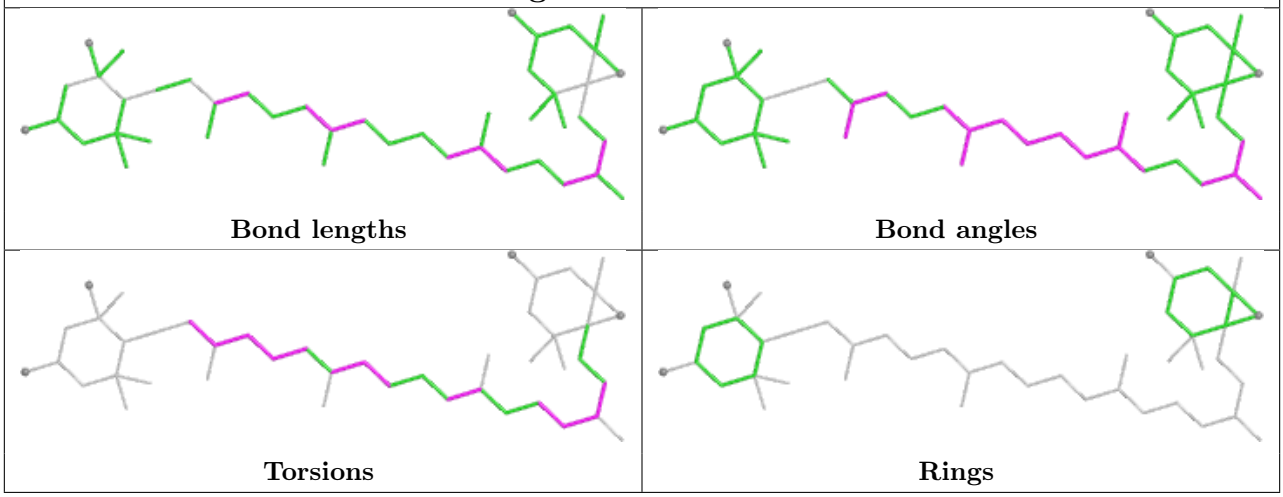
Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

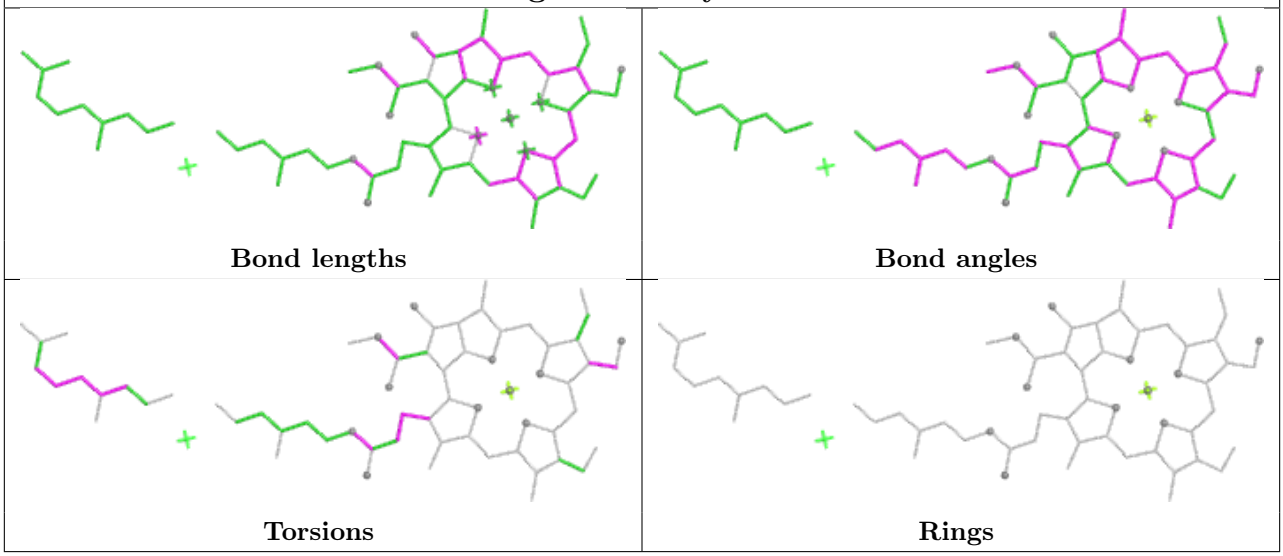
Ligand CLA 8 301



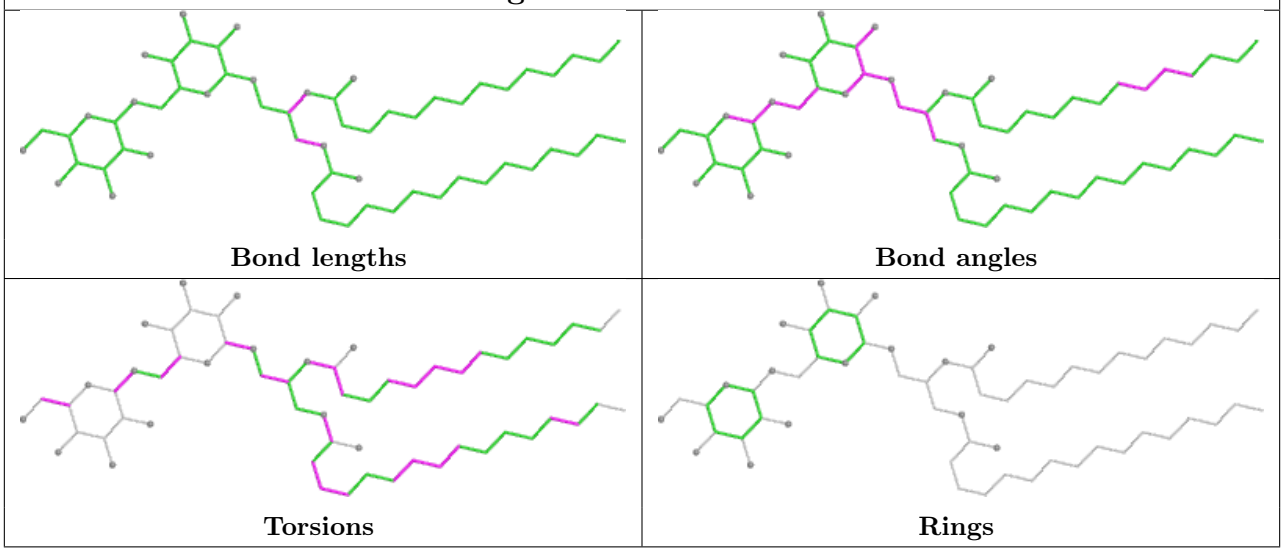
Ligand NEX s 616



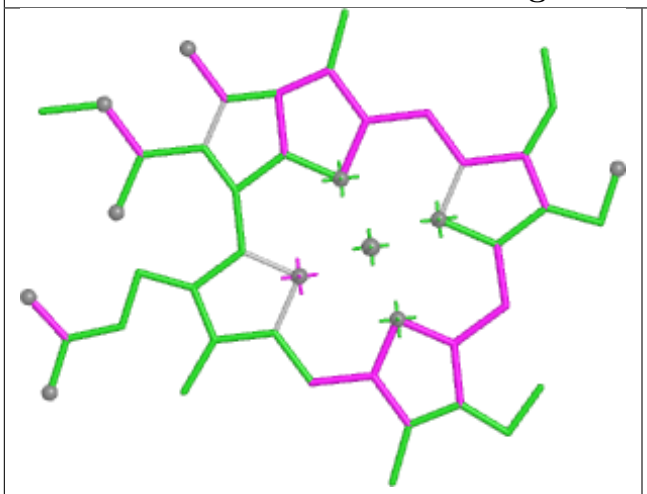
Ligand CHL y 309



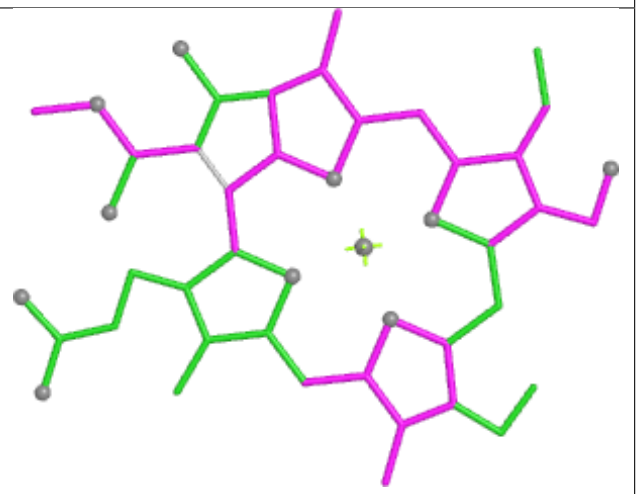
Ligand DGD BD 413



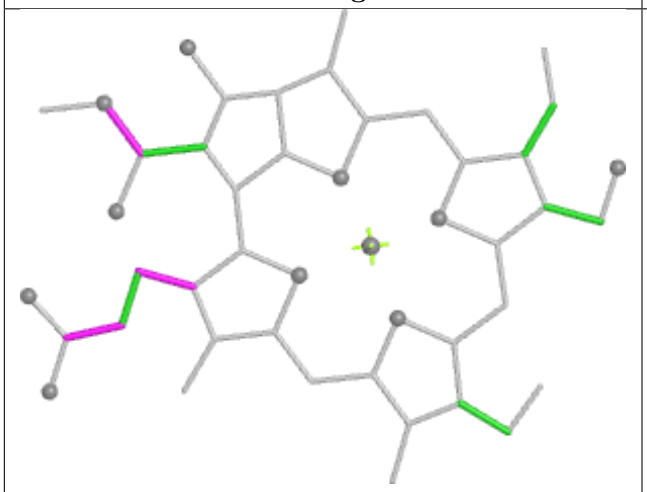
Ligand CHL 7 307



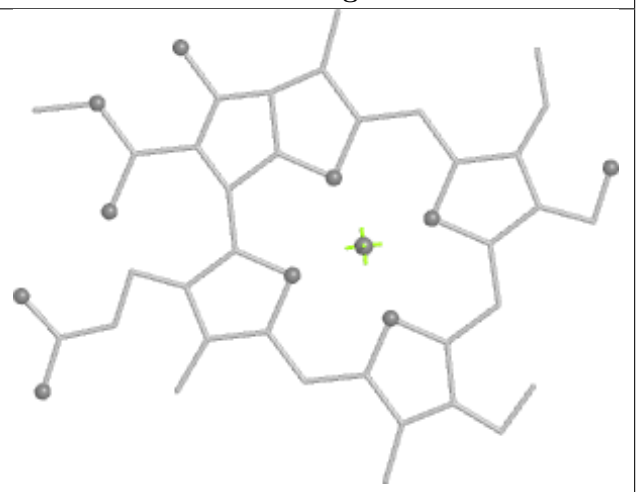
Bond lengths



Bond angles

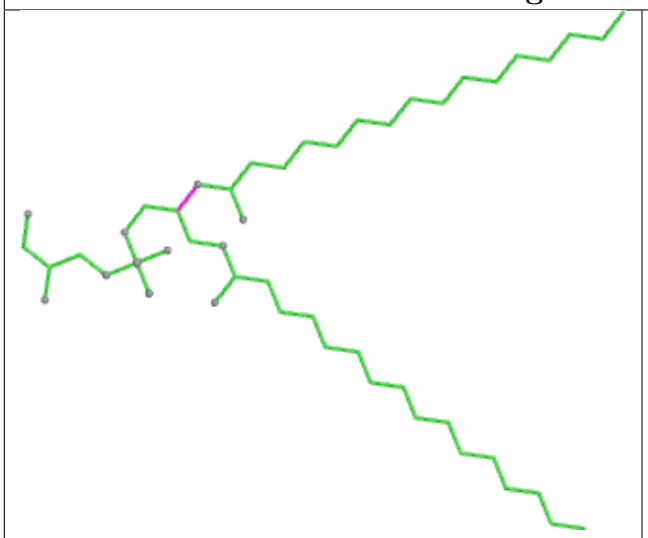


Torsions



Rings

Ligand LHG L 102



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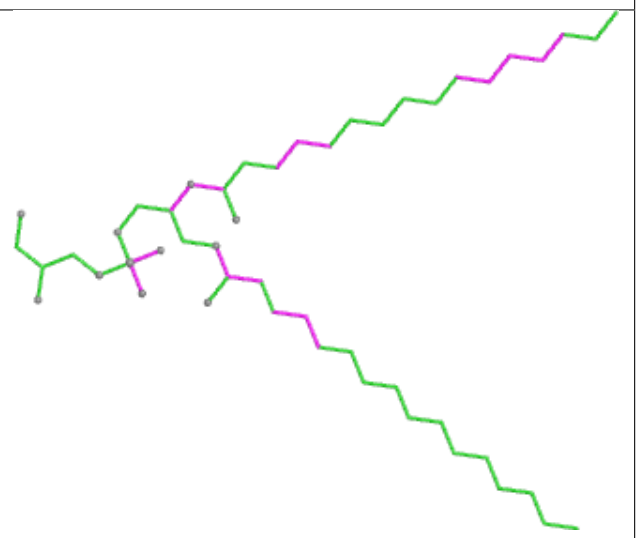
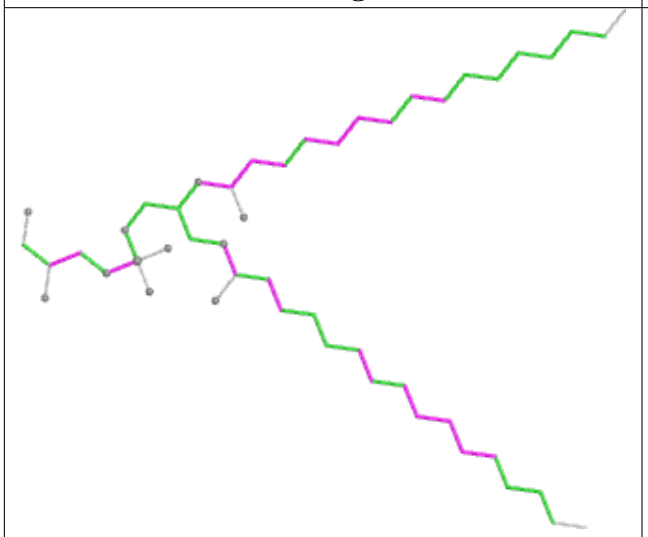


Bond angles



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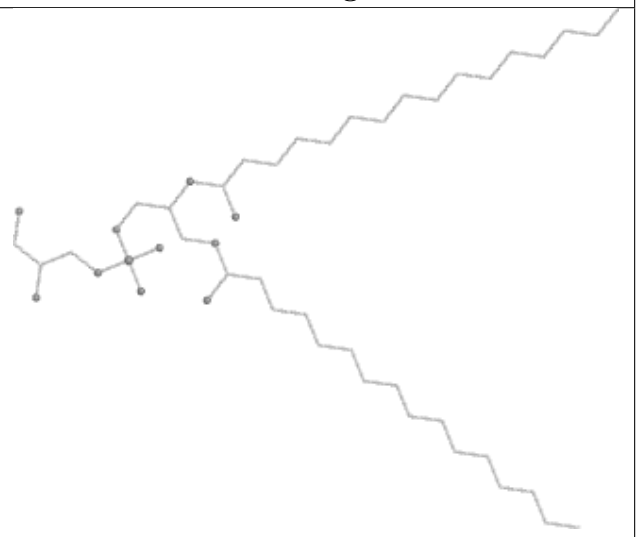
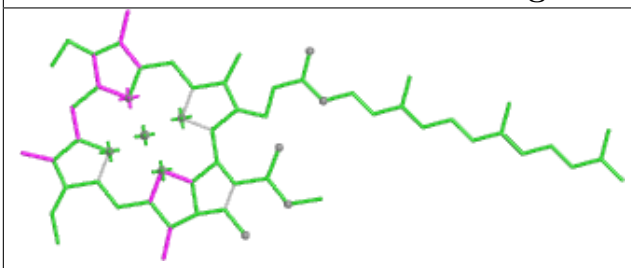
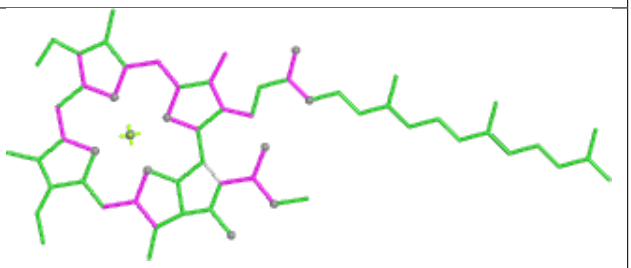
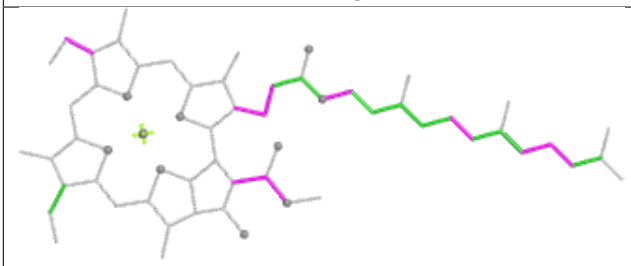
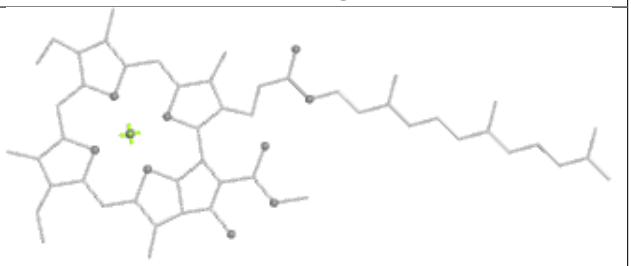
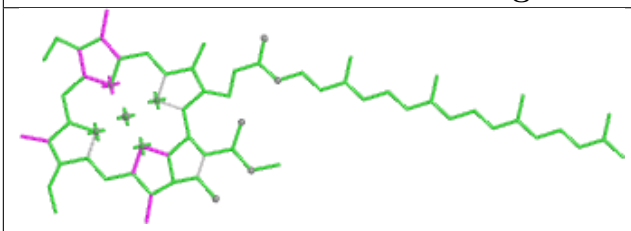
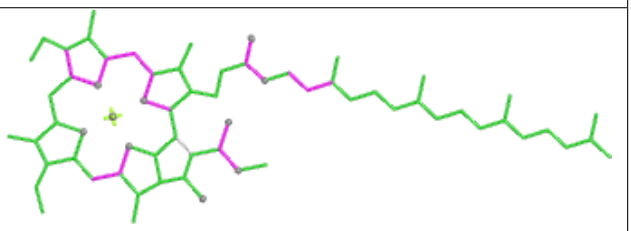
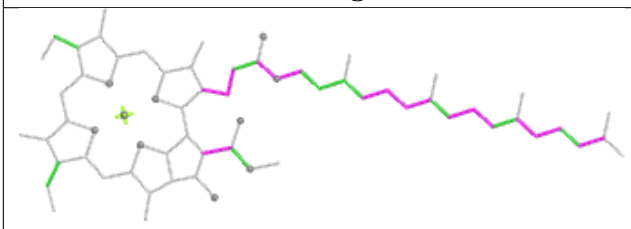
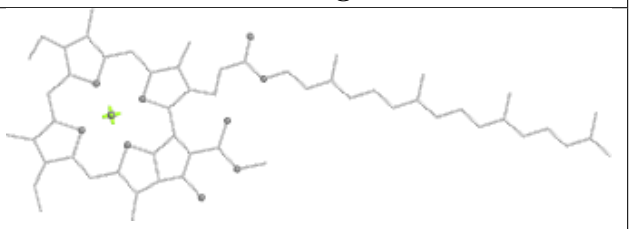


Rings

Ligand CLA 0 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BE 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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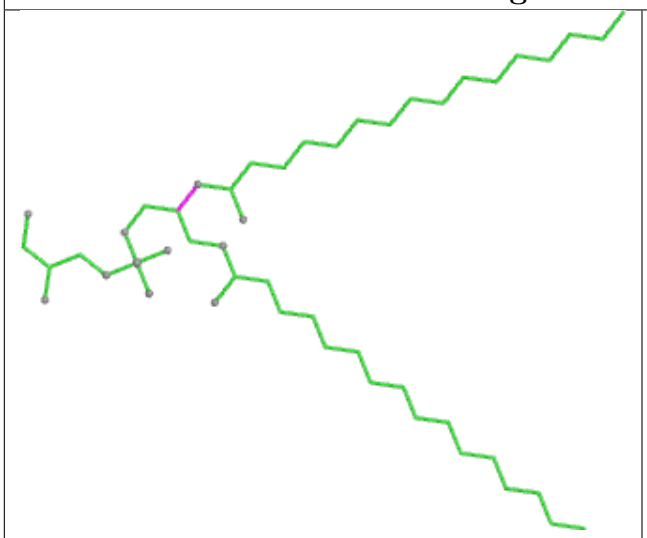
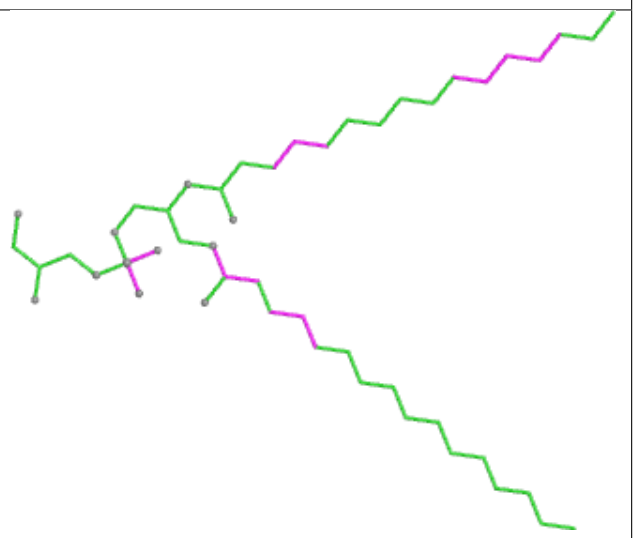
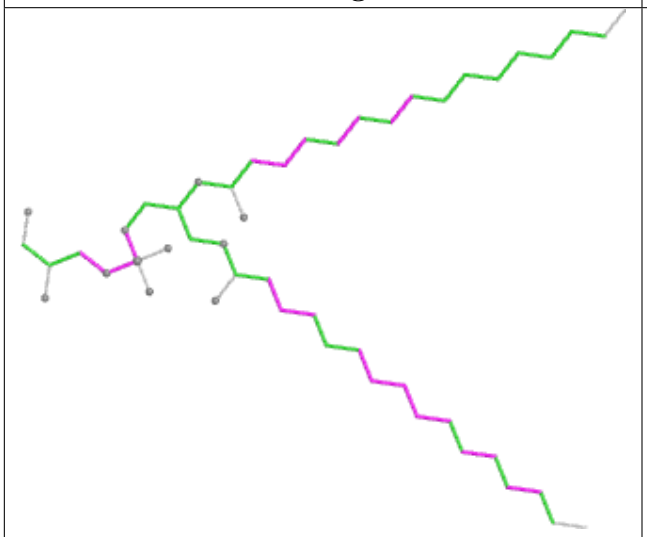
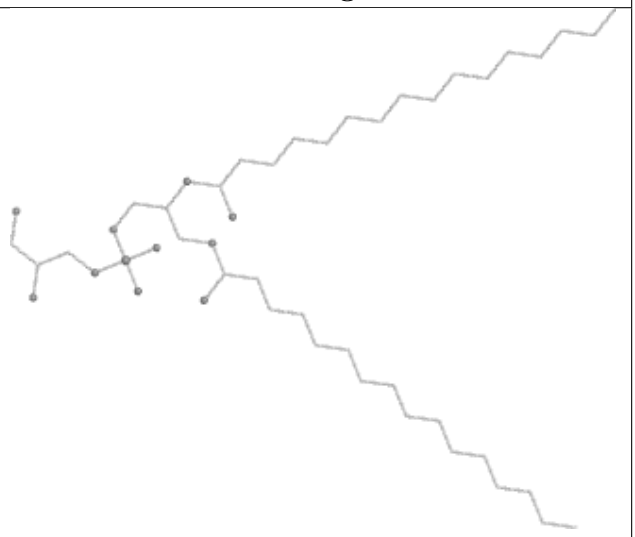
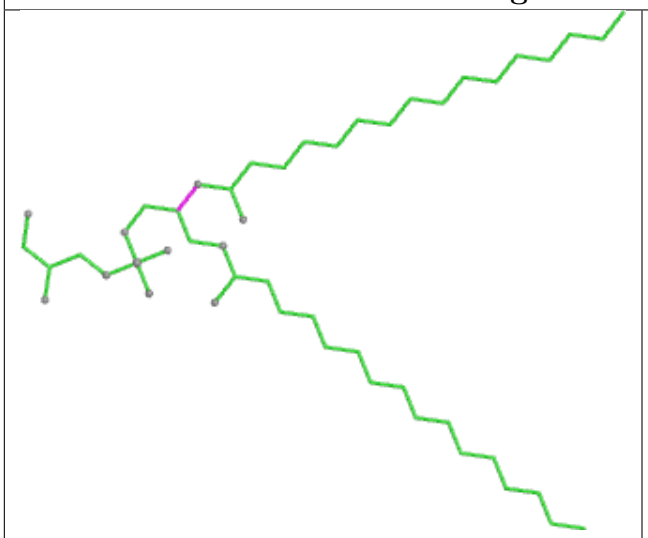
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG BY 201



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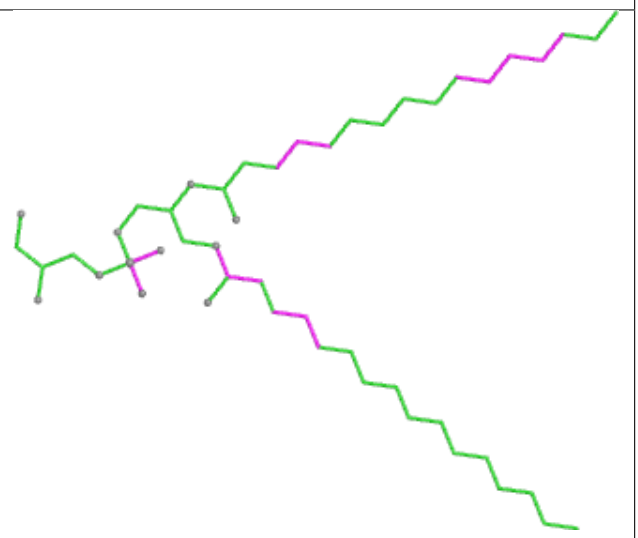

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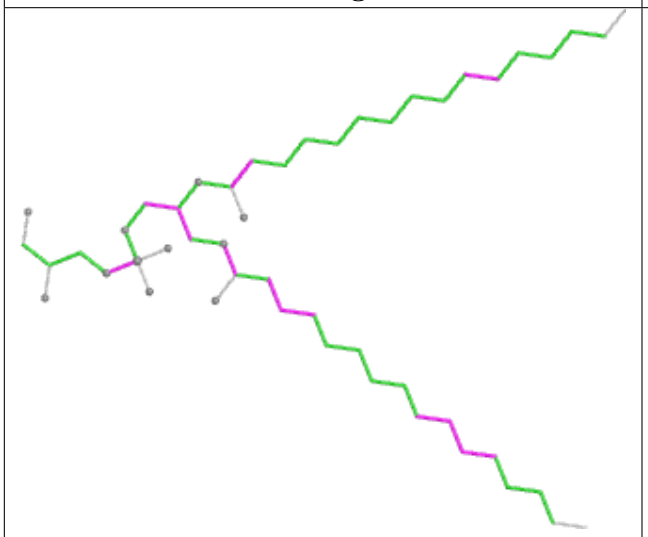

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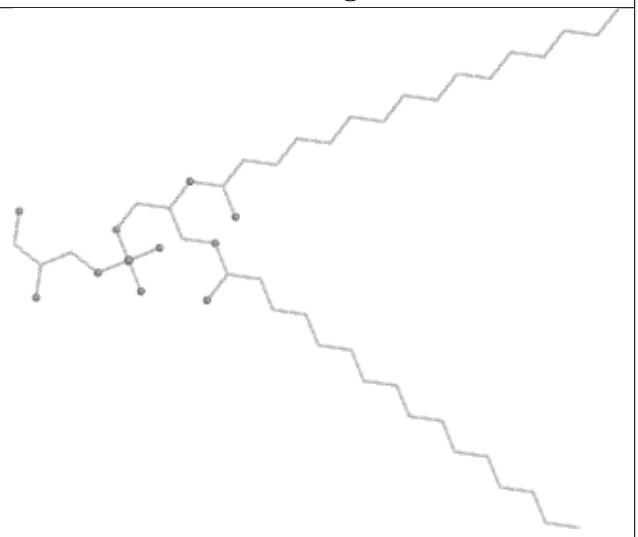
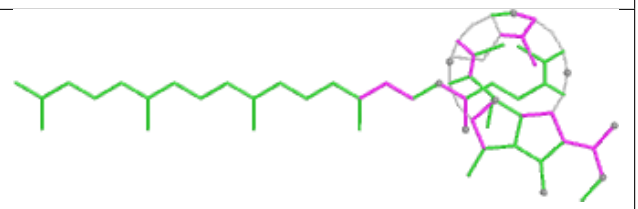


Rings

Ligand PHO R 407

Bond lengths



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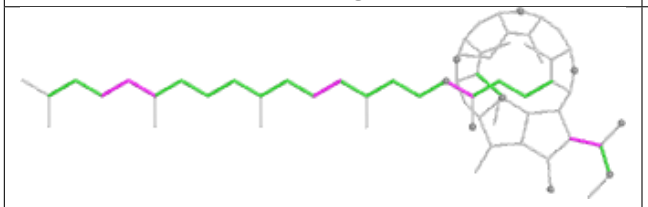

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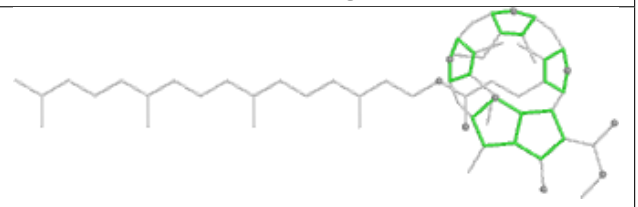
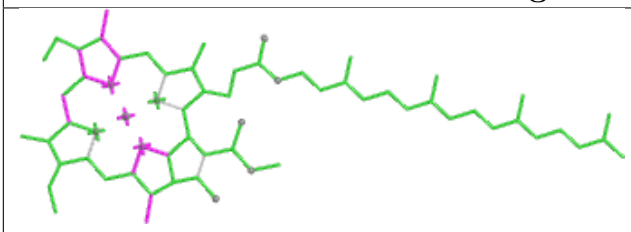
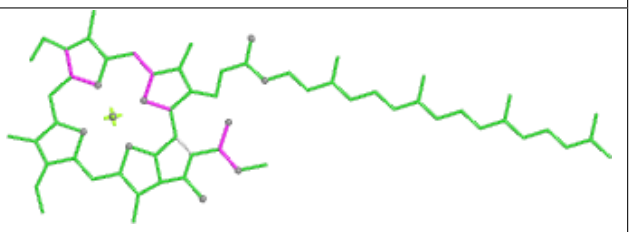
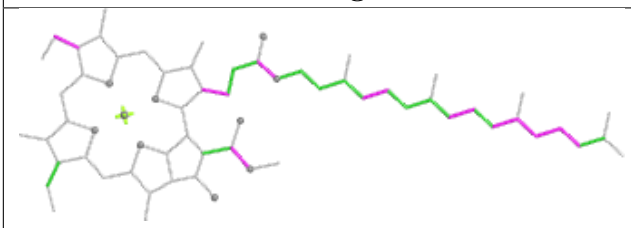
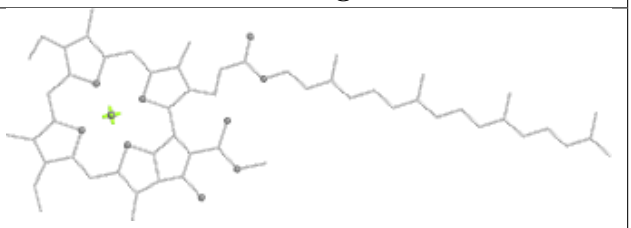


Rings

Ligand CLA c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

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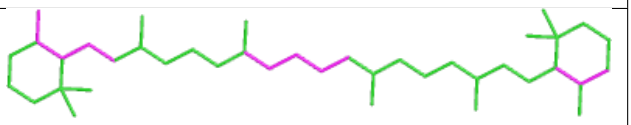
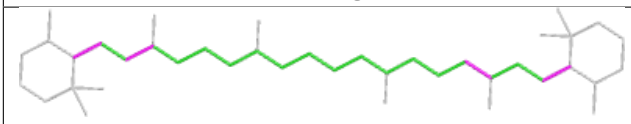
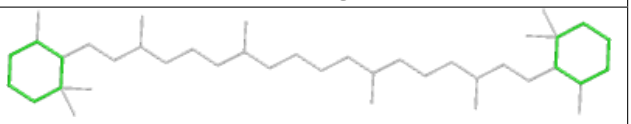
Bond lengths	 Bond angles
 Torsions	 Rings

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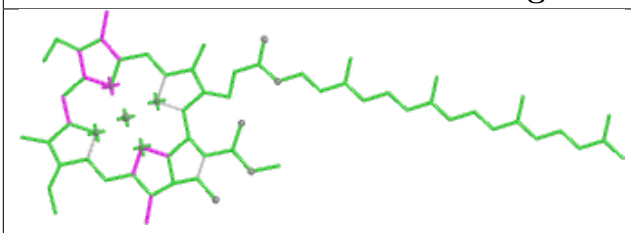
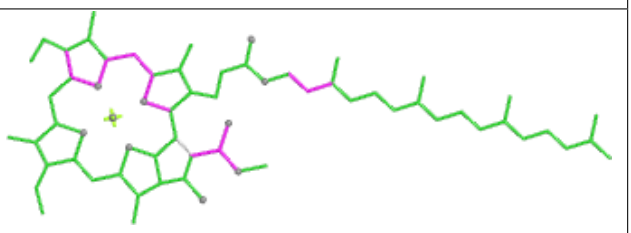
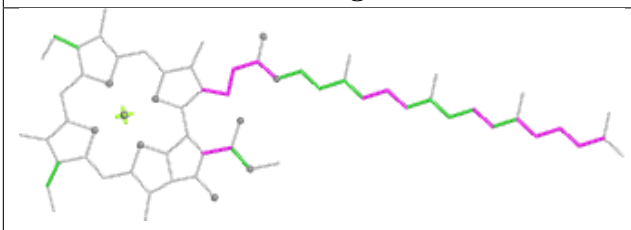
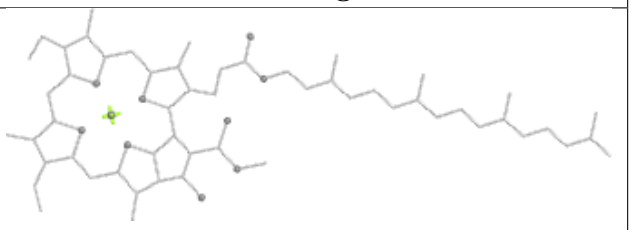
 Bond lengths	 Bond angles
 Torsions	 Rings

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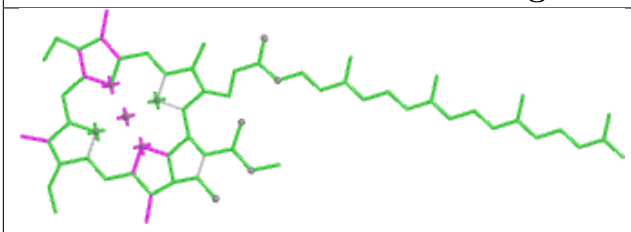
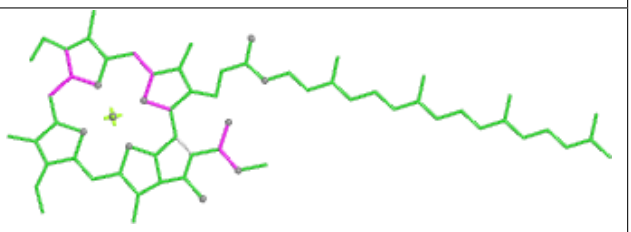
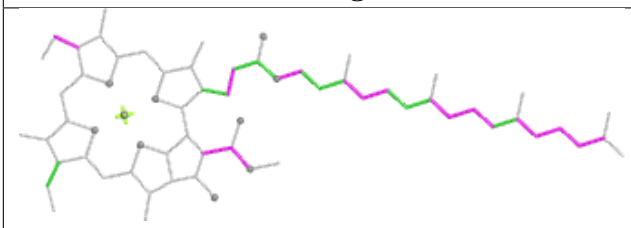
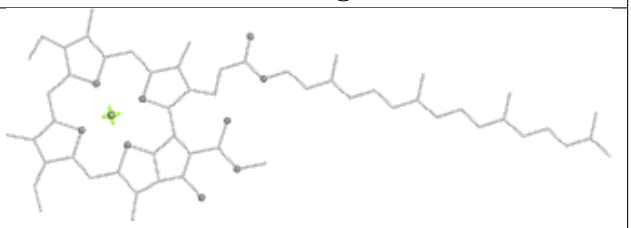
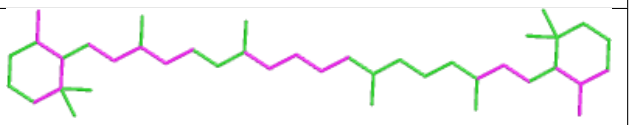
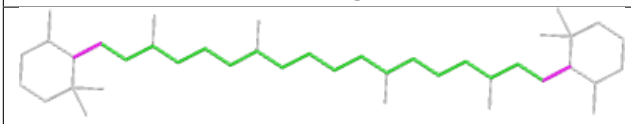
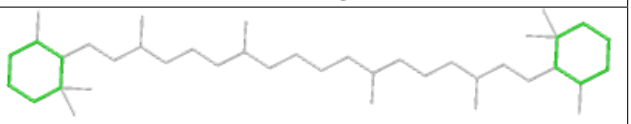
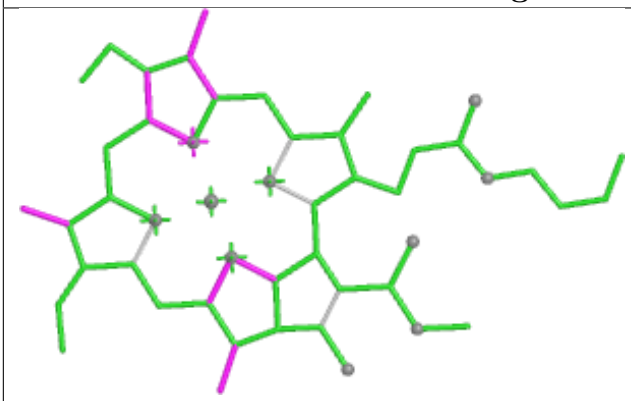
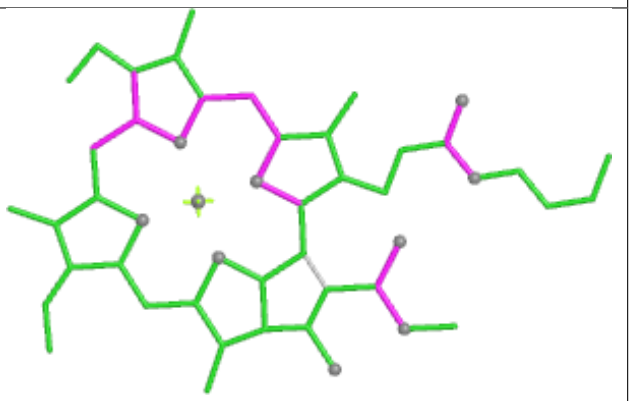
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR Av 101	
Bond lengths	 Bond angles
 Torsions	 Rings

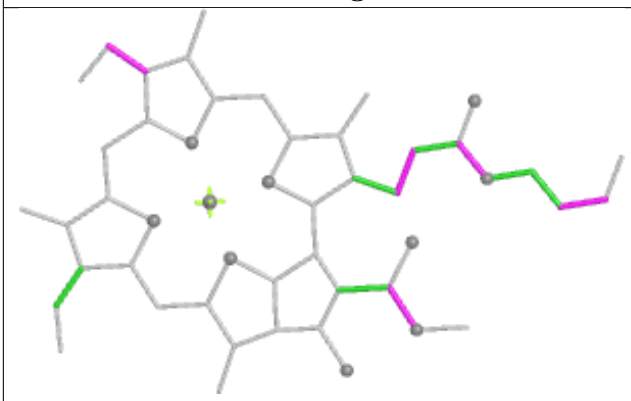
Ligand CLA BV 613



Bond lengths



Bond angles



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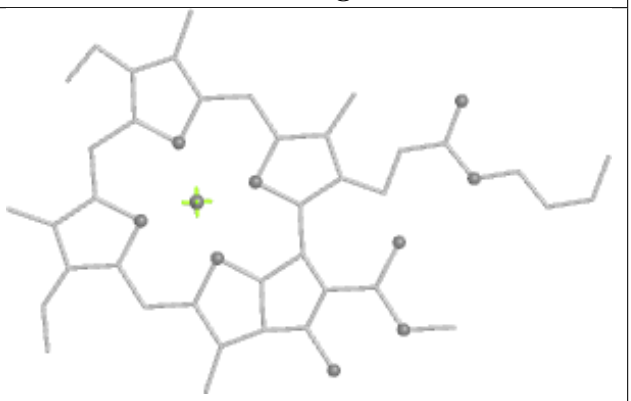
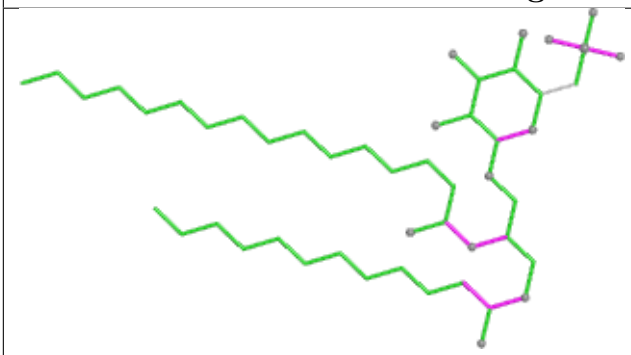


Rings

Ligand SQD d 406



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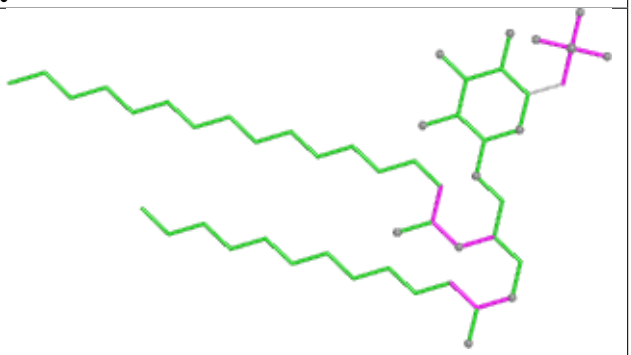
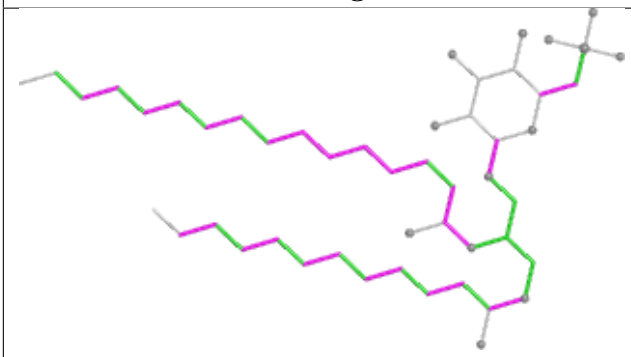


Bond angles



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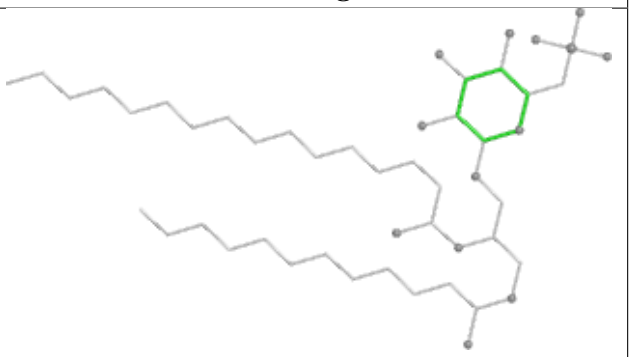
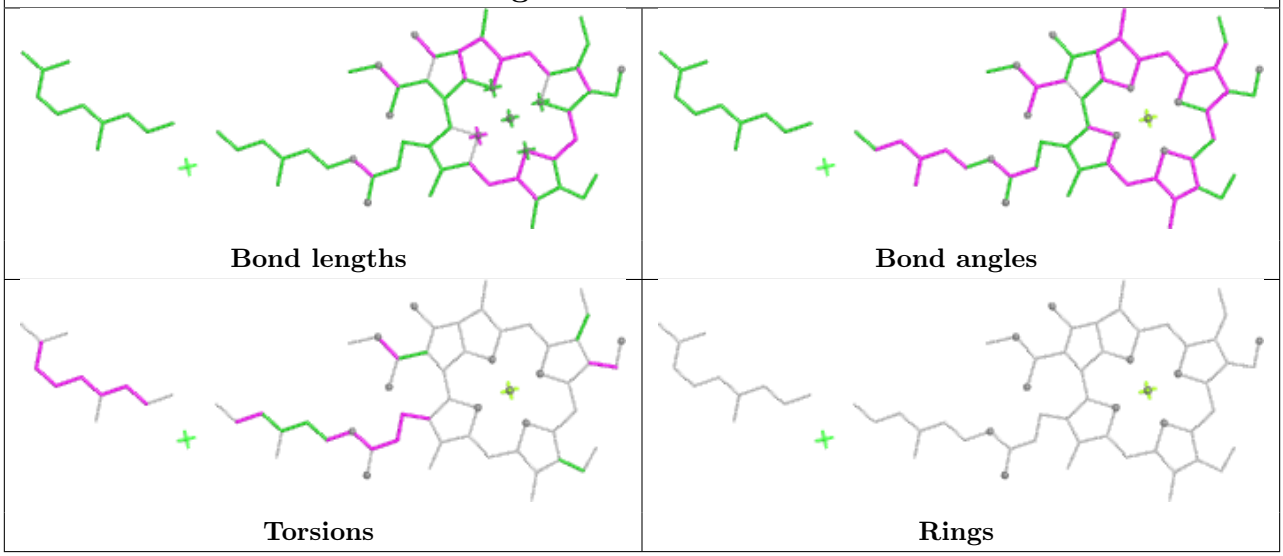
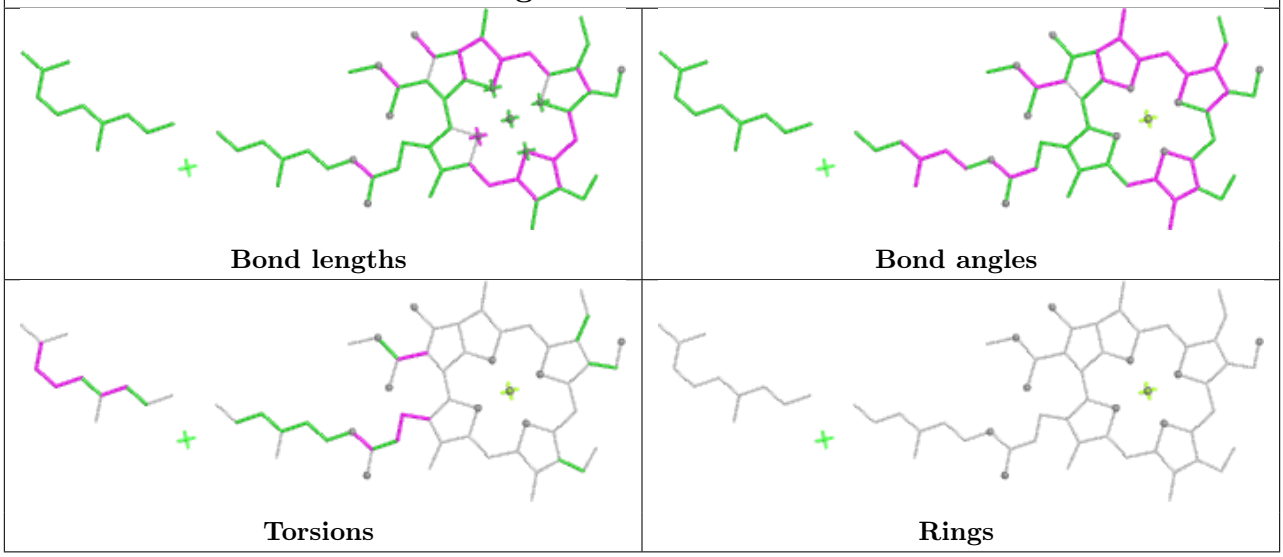


Rings

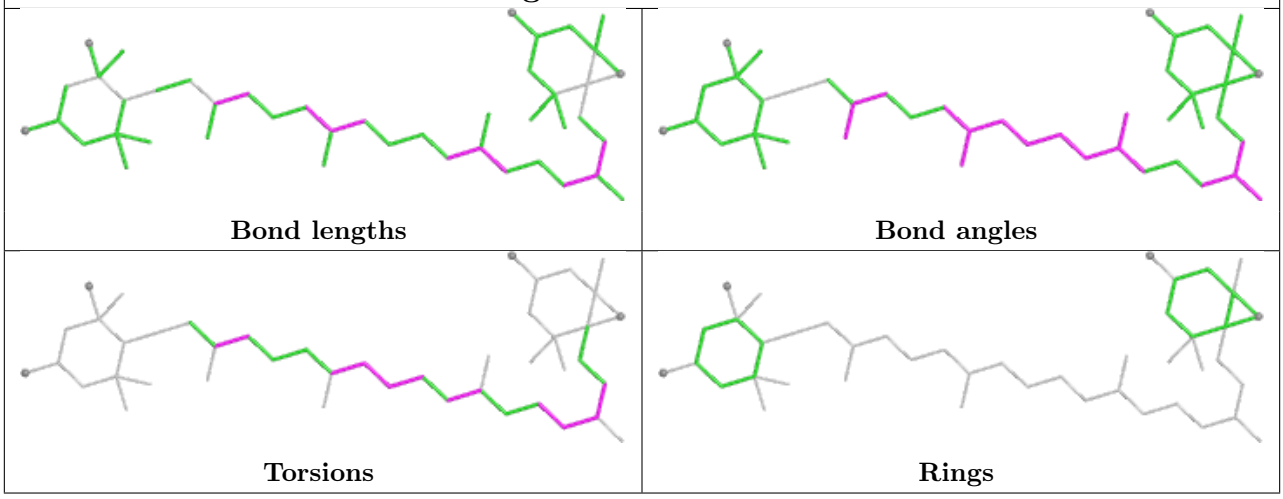
Ligand CHL BU 605



Ligand CHL A2 609



Ligand NEX Y 318



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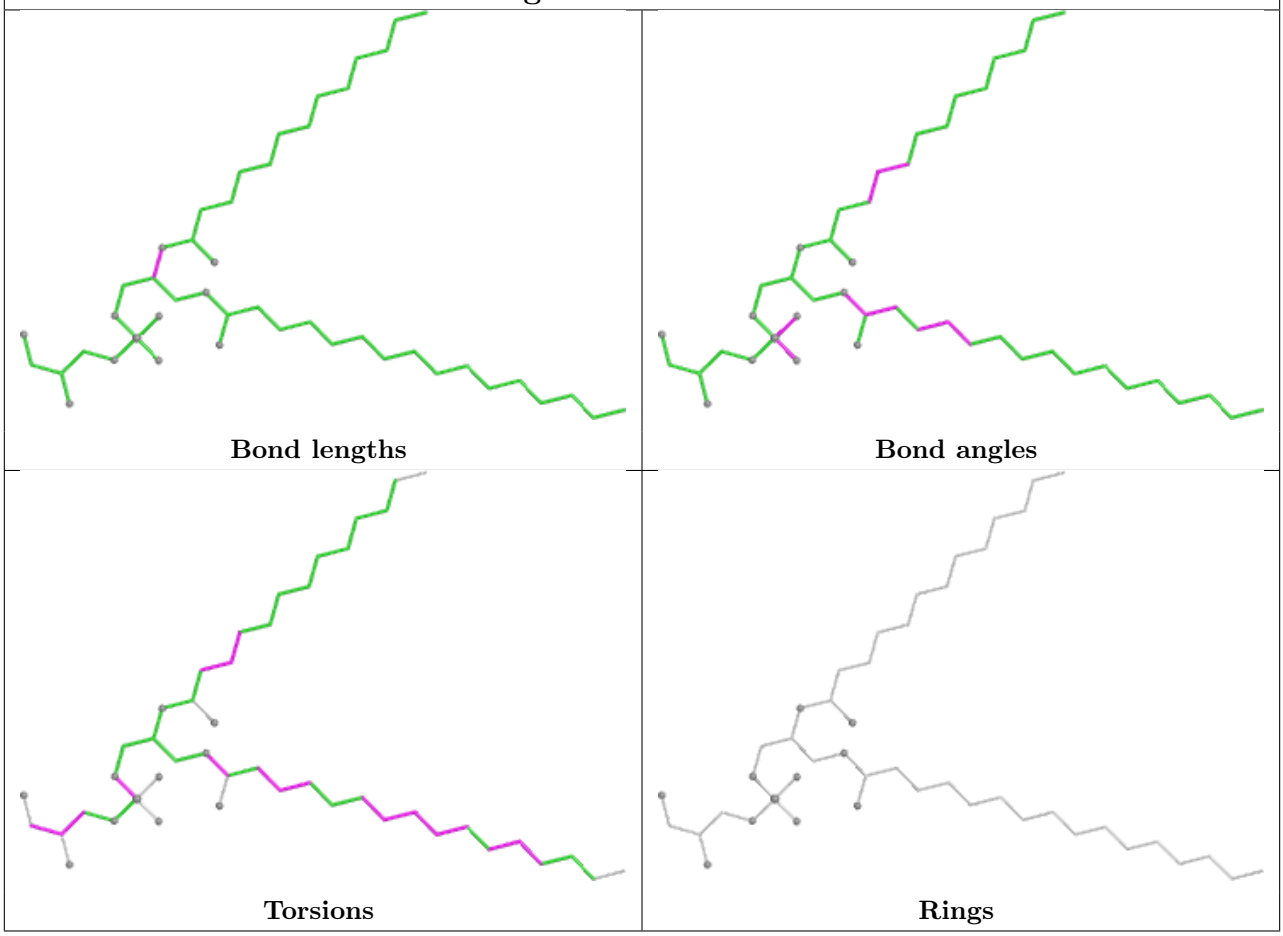

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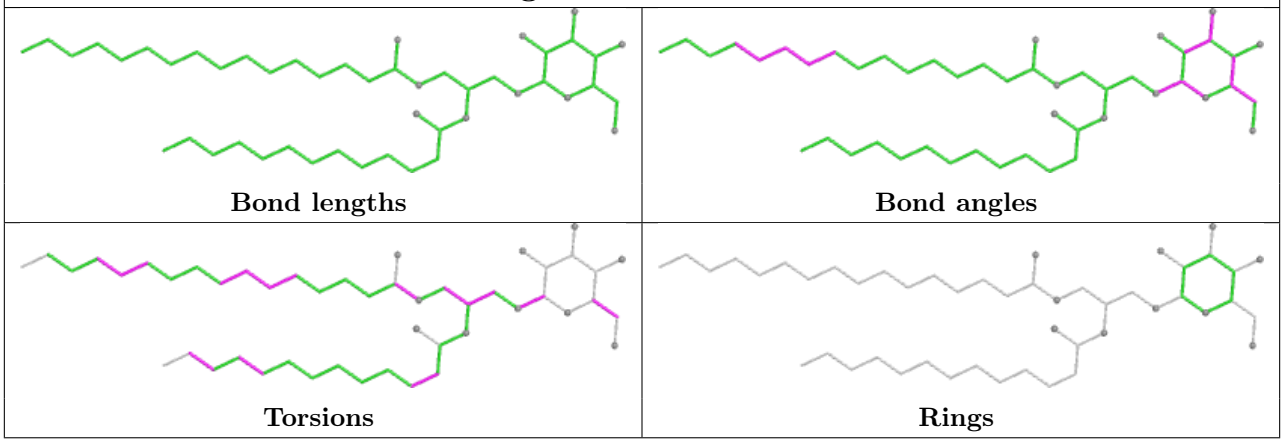
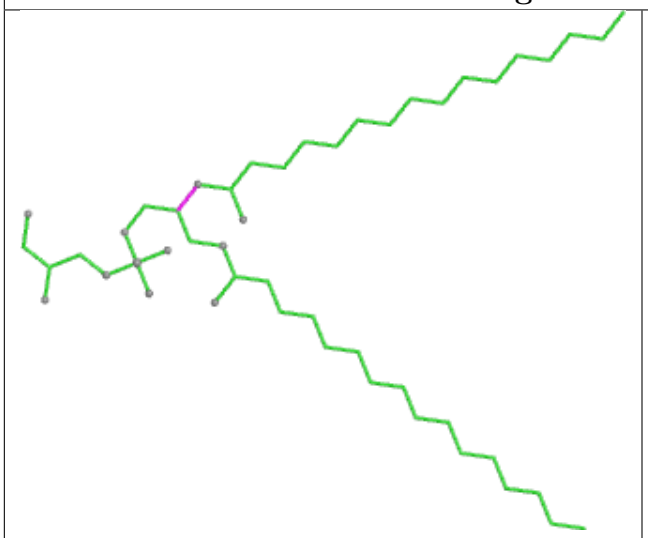
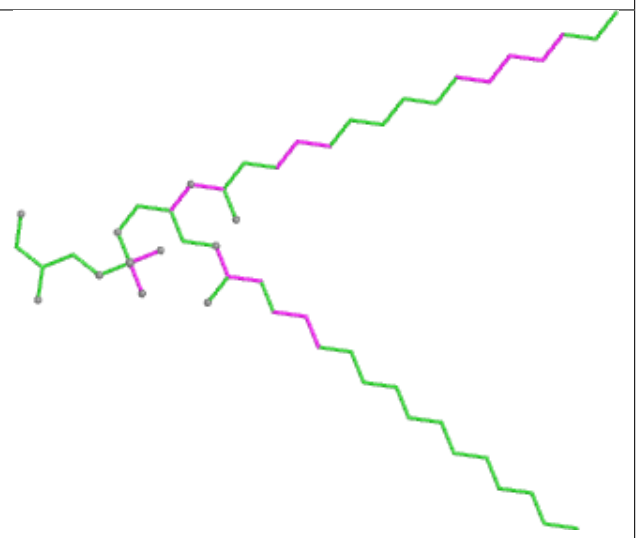


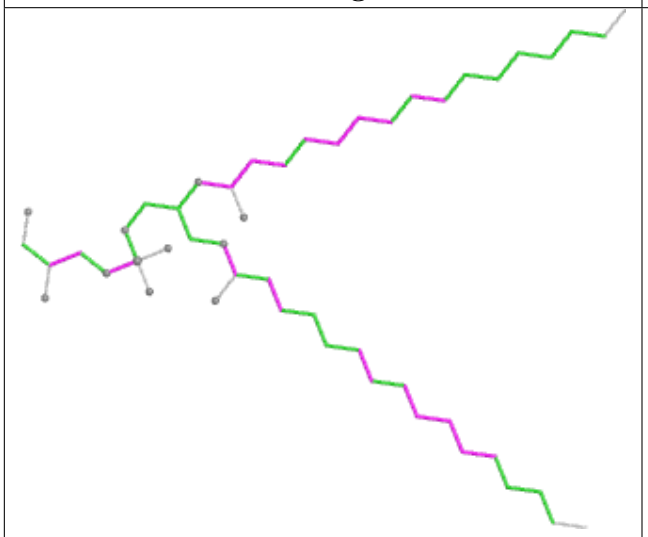
Ligand LHG Az 102



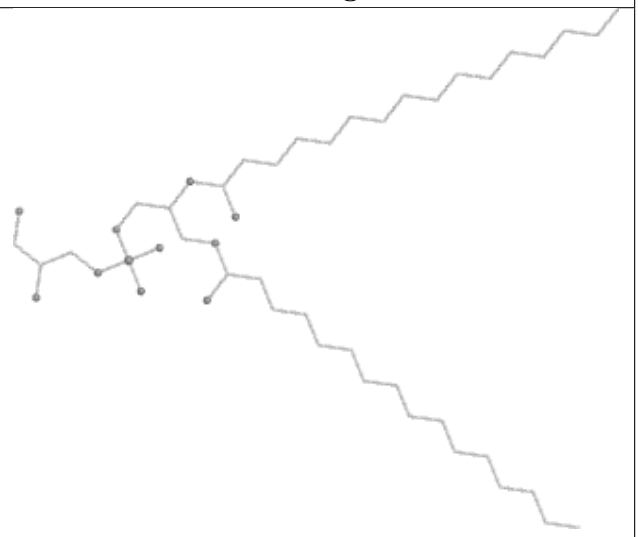
Bond lengths



Bond angles

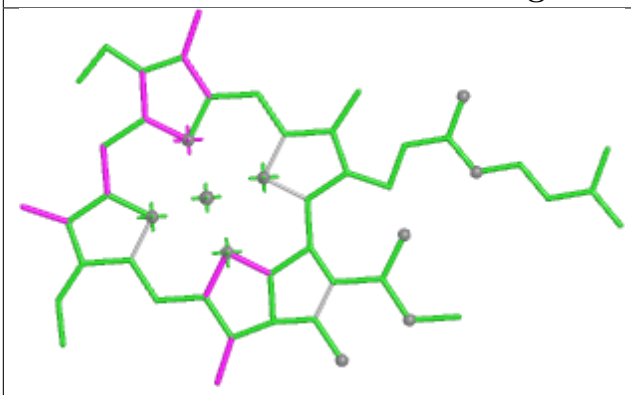


Torsions



Rings

Ligand CLA y 305



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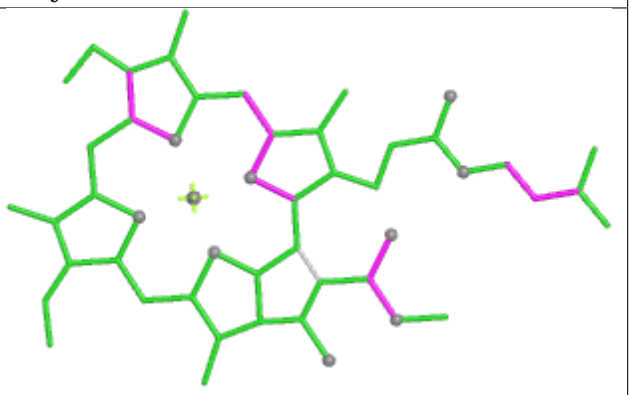
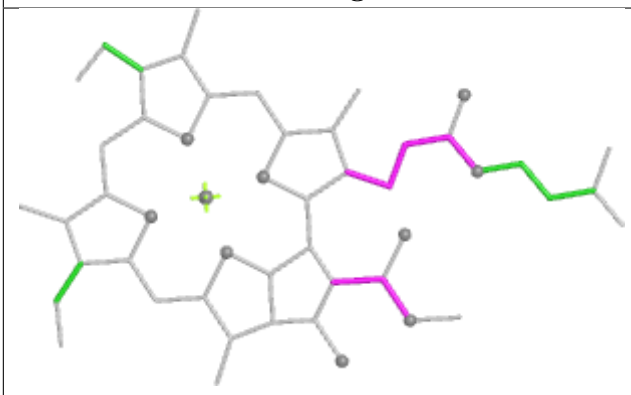


Bond angles



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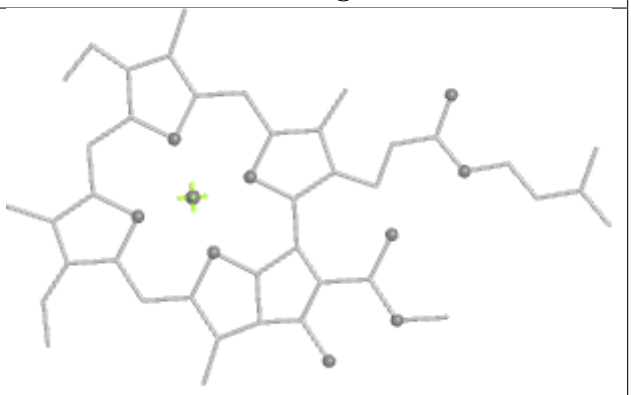
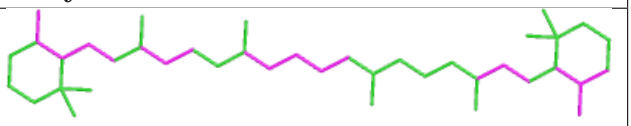


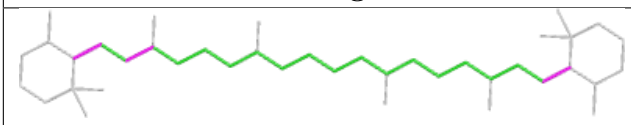
Rings

Ligand BCR Ay 102

Bond lengths



Bond angles



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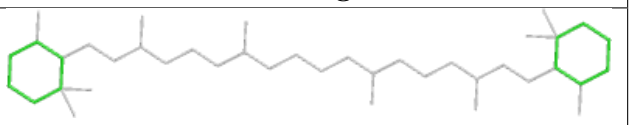
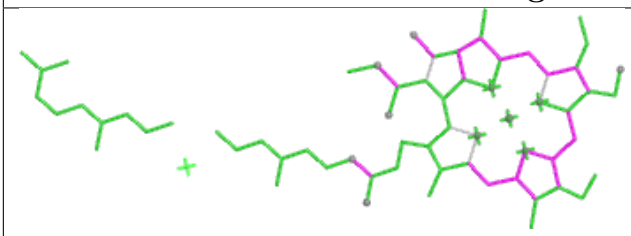
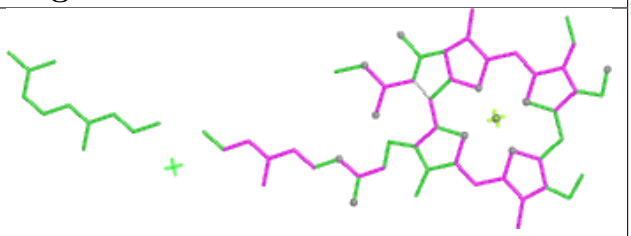
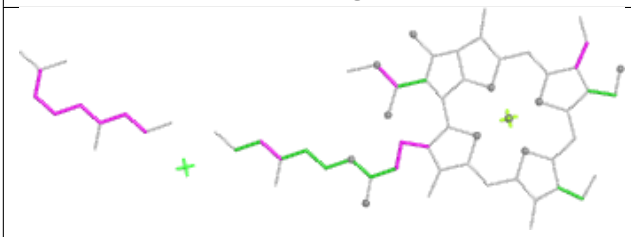
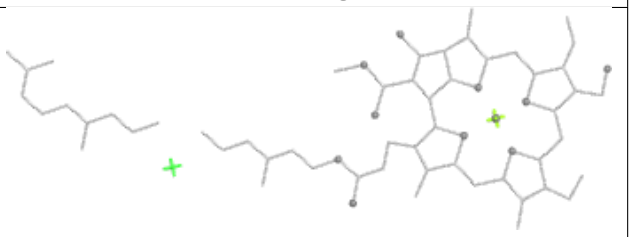


Rings

Ligand CHL g 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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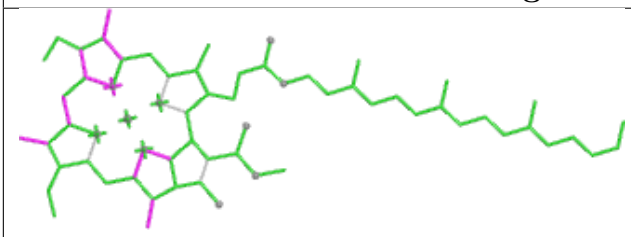
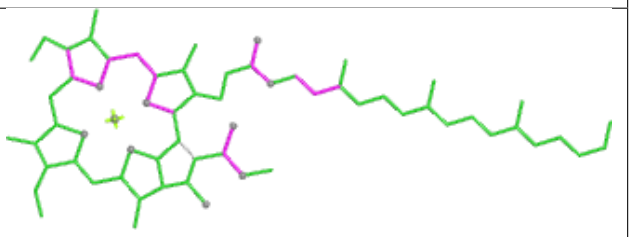
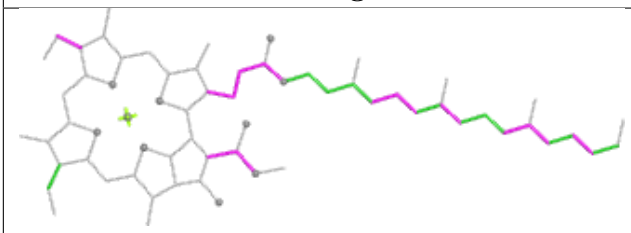
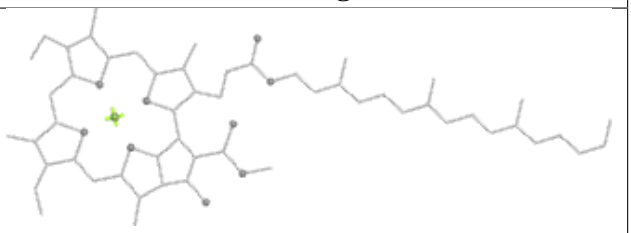
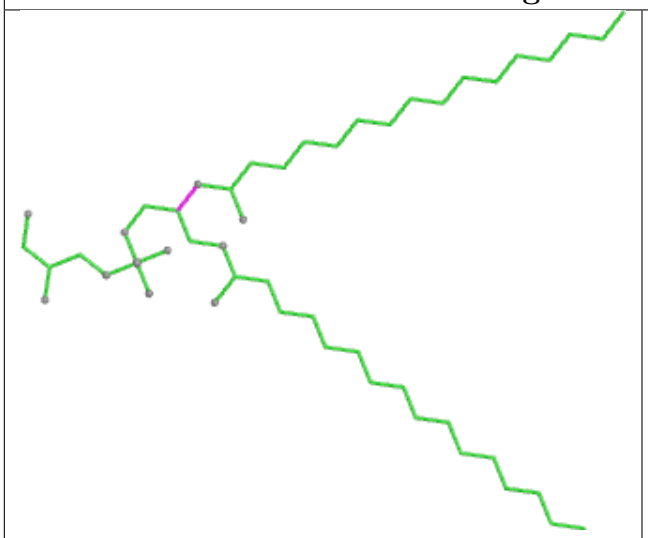
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG N 618



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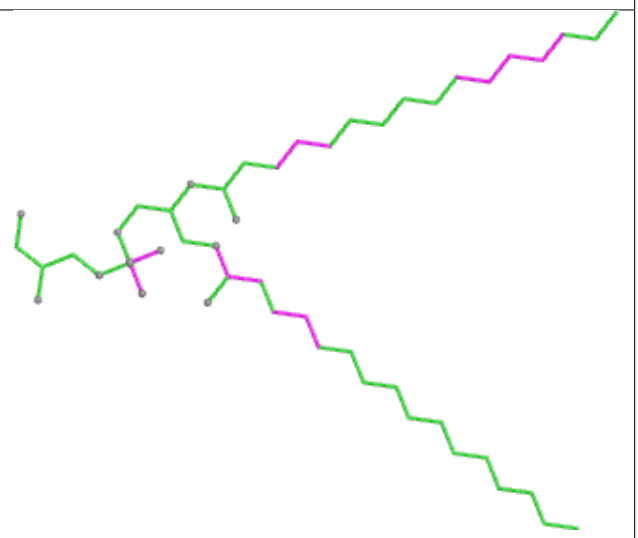

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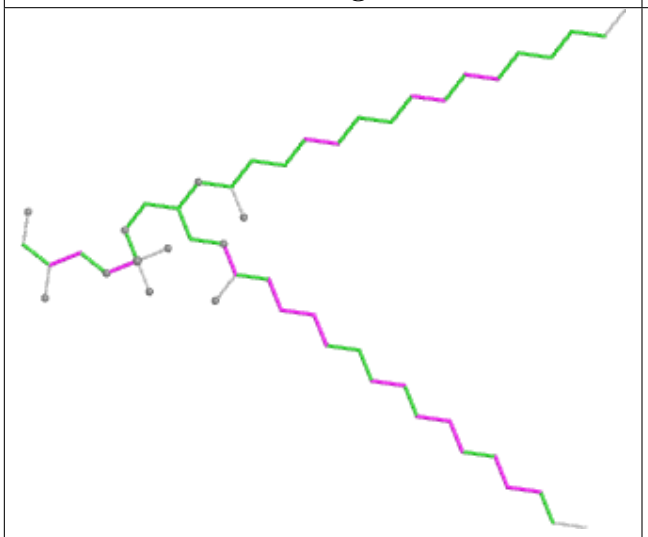

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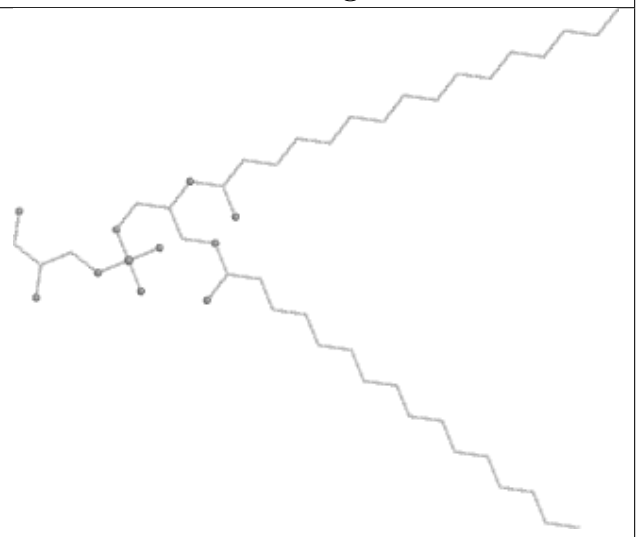

Rings

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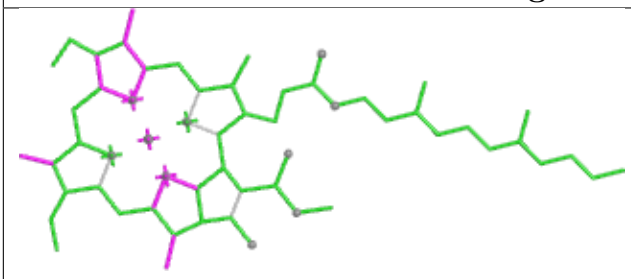
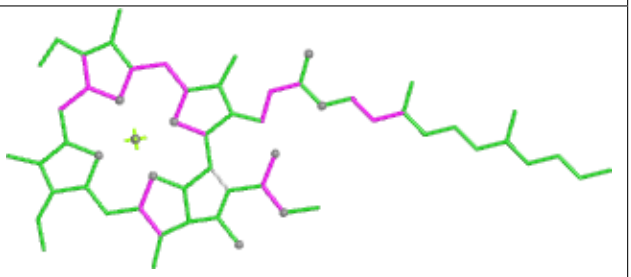
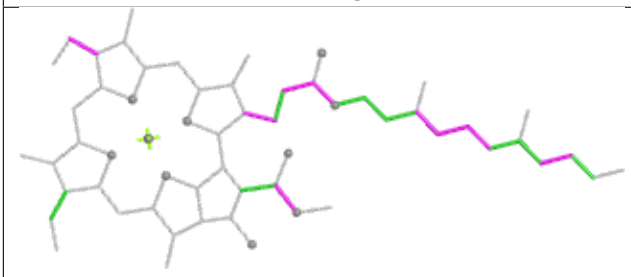
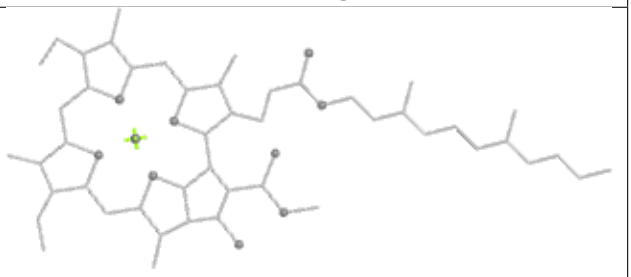
 Bond lengths	 Bond angles
 Torsions	 Rings

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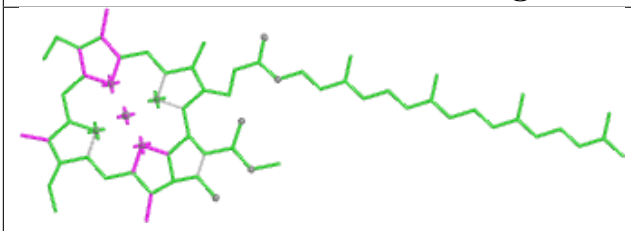
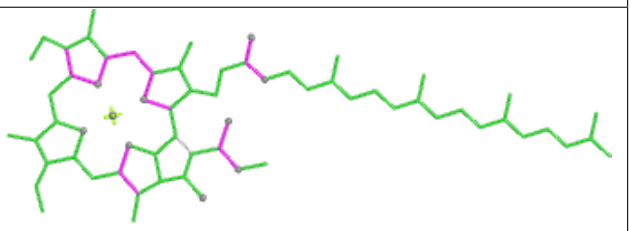
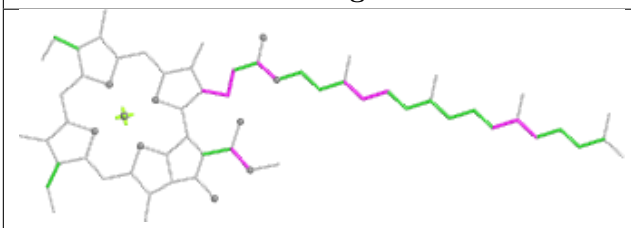
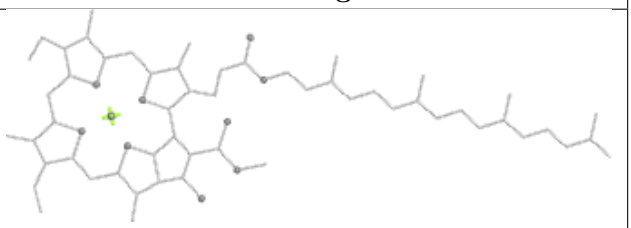
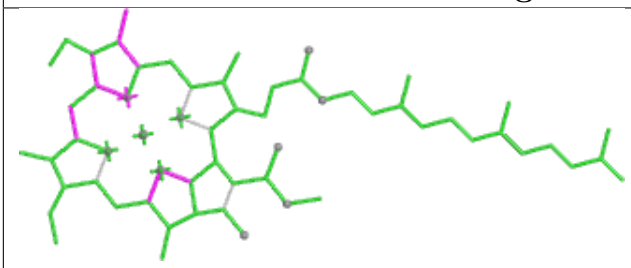
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BJ 611



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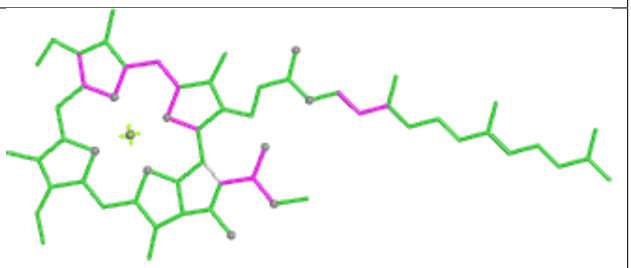

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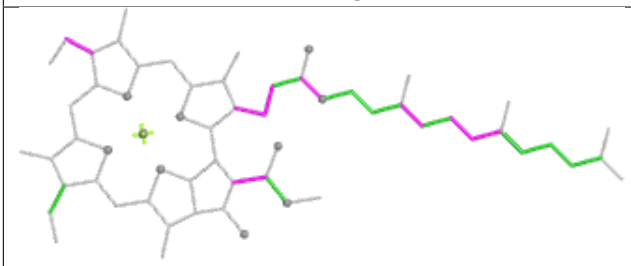

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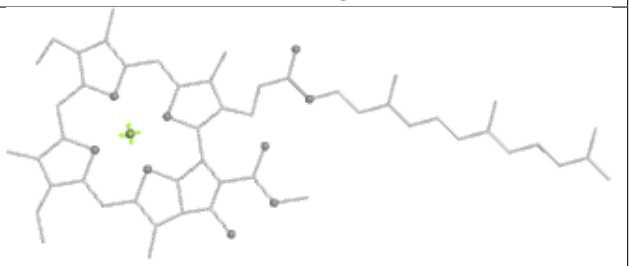
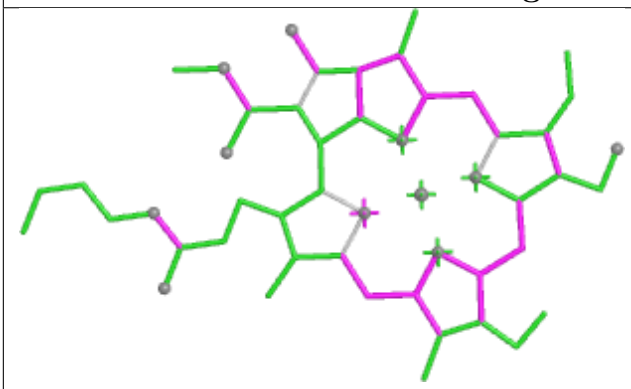


Rings

Ligand CHL N 606



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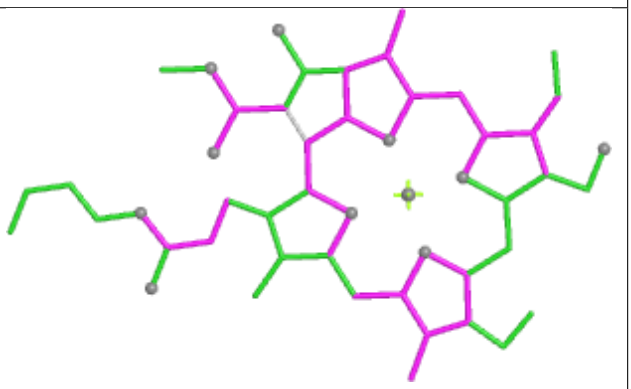

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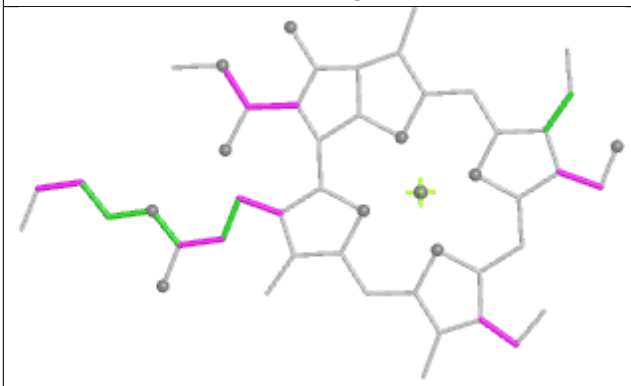

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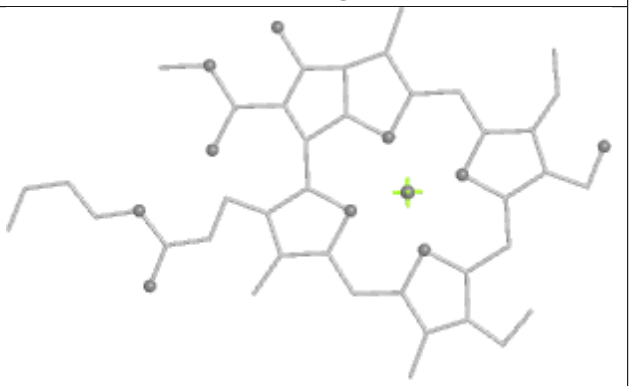
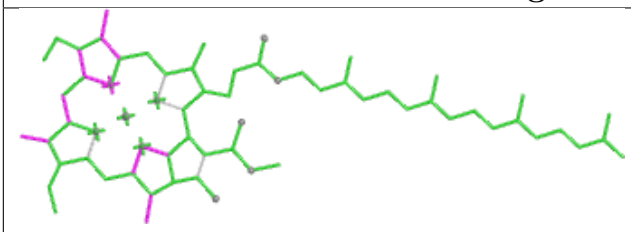
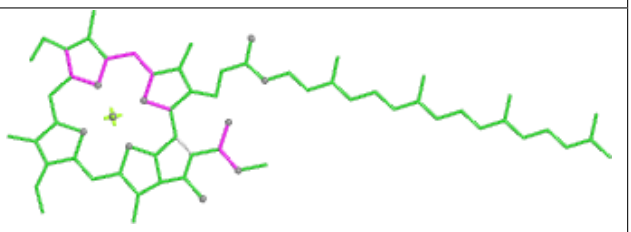
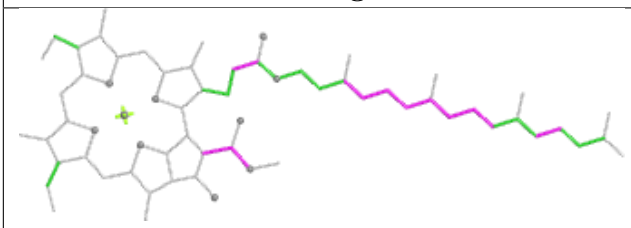
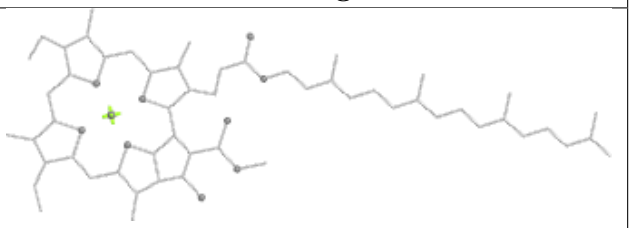


Rings

Ligand CLA v 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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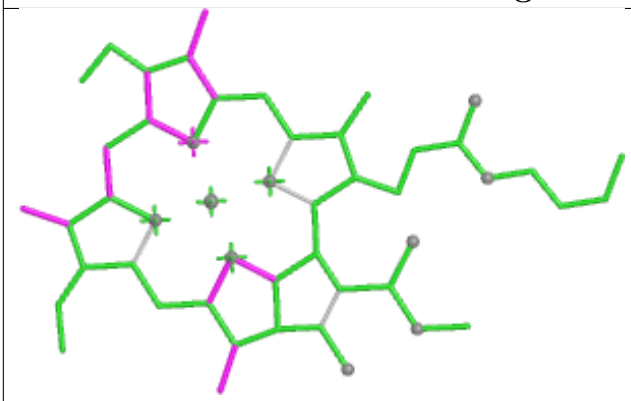
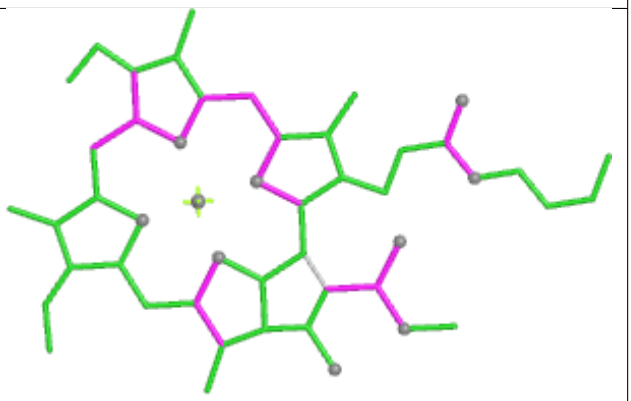
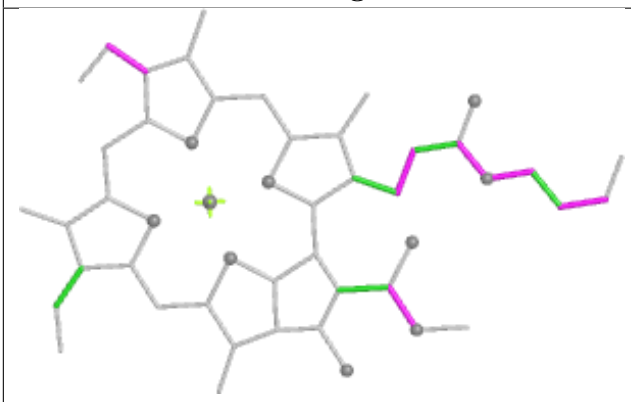
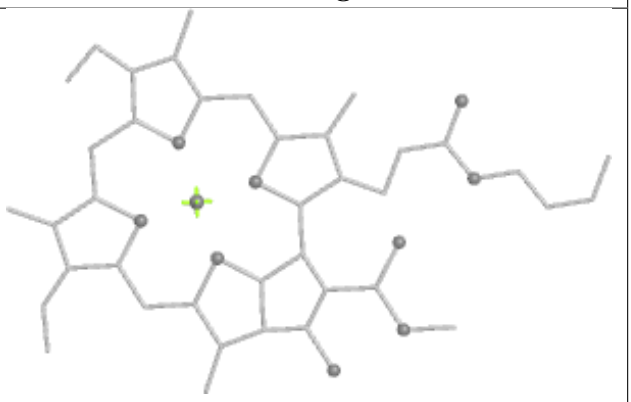
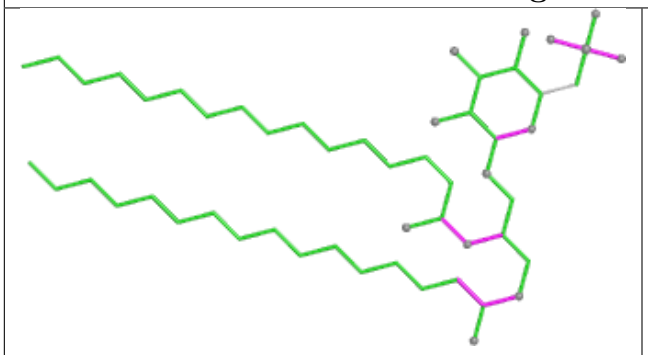
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 412



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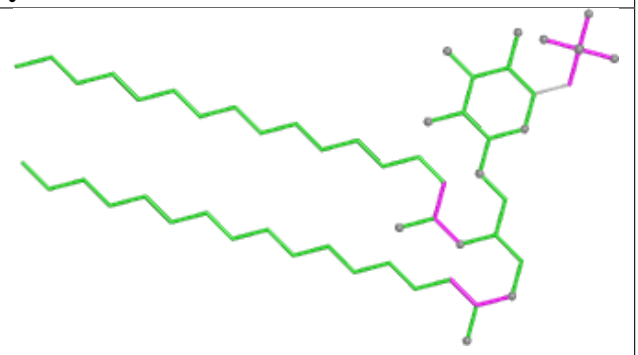

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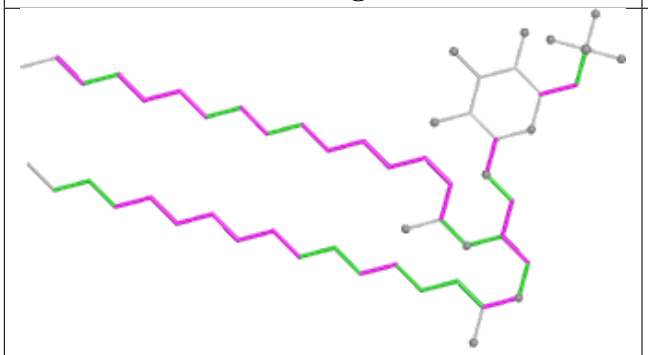

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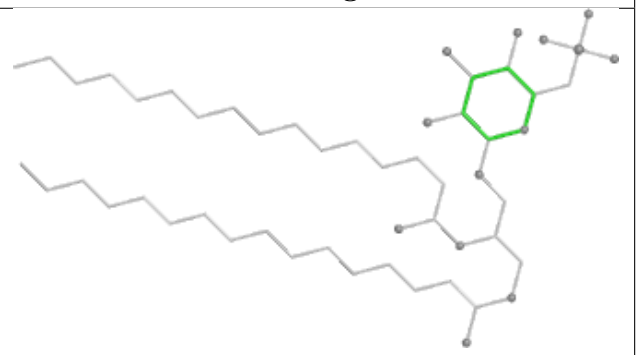
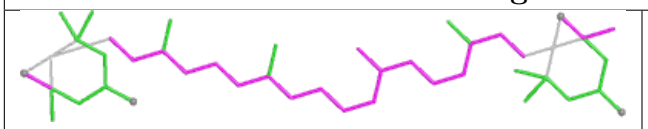


Rings

Ligand XAT AA 318



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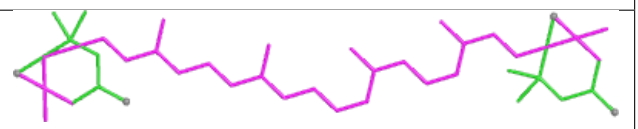

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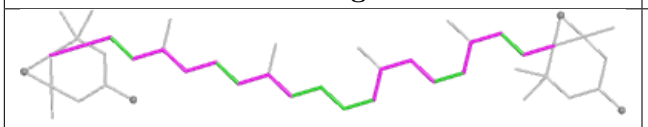

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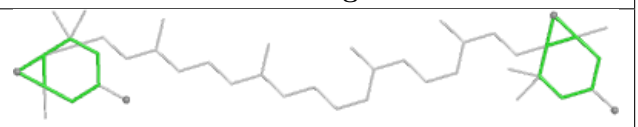
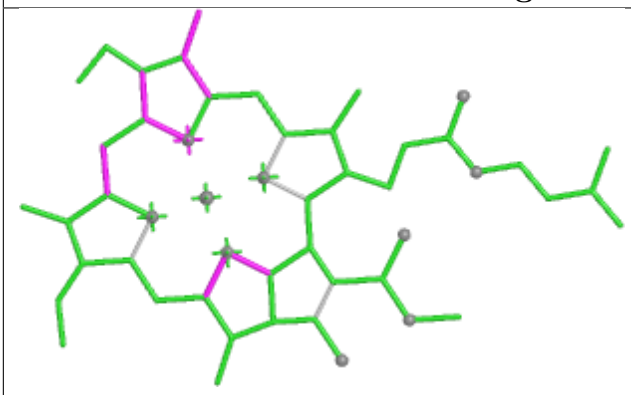
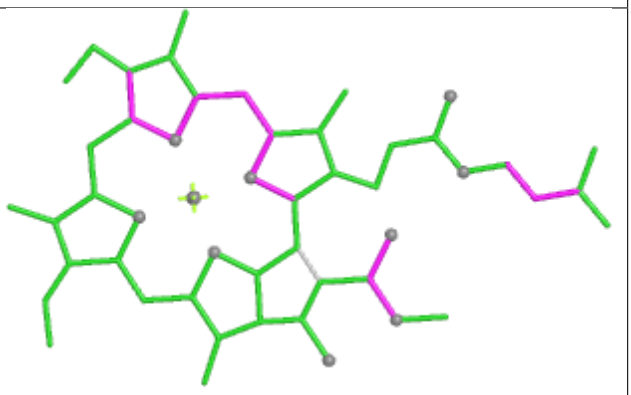
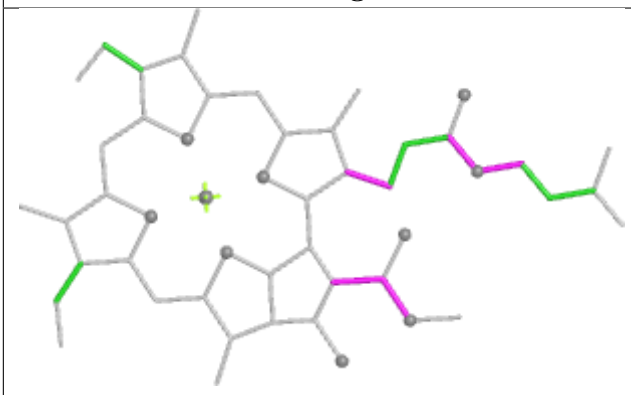
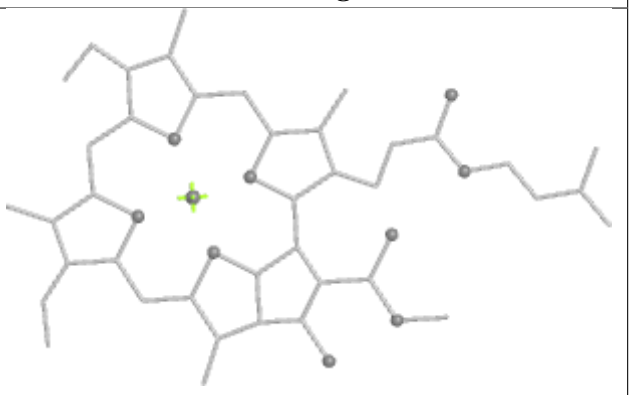
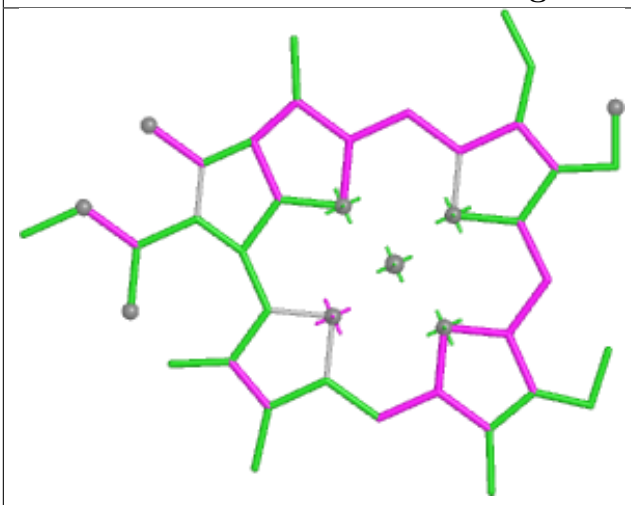


Rings

Ligand CLA BJ 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 613



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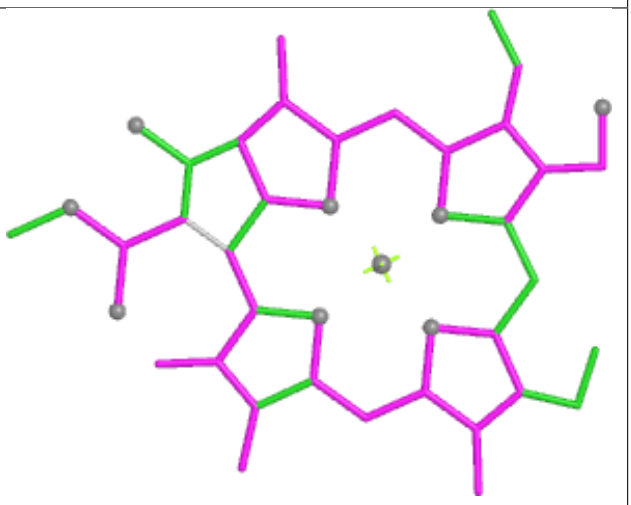

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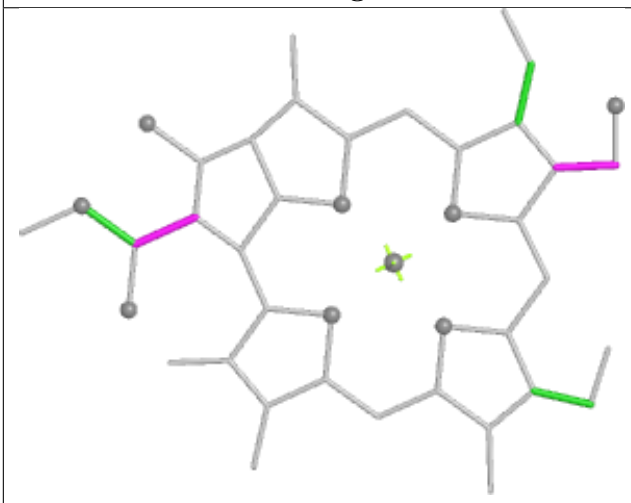

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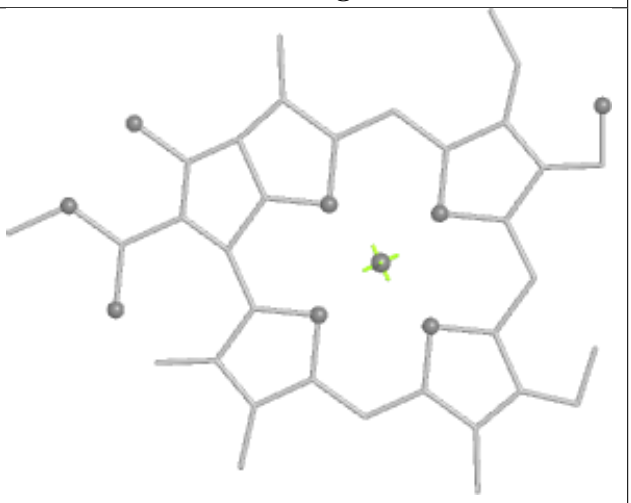
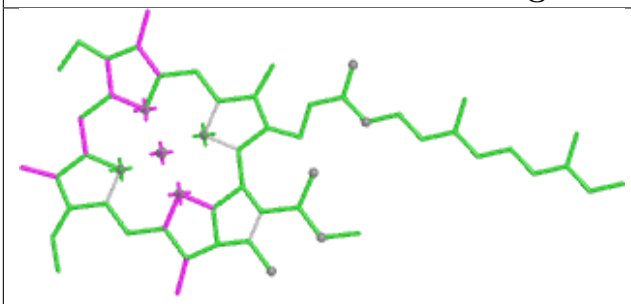


Rings

Ligand CLA 9 610



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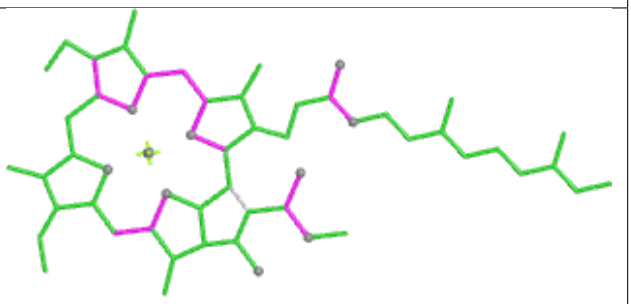
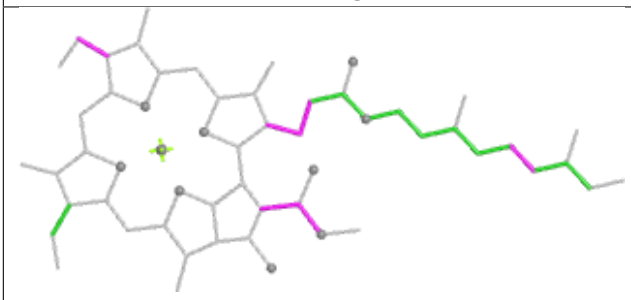


Bond angles



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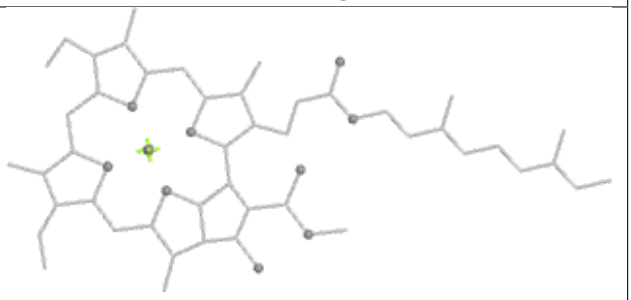
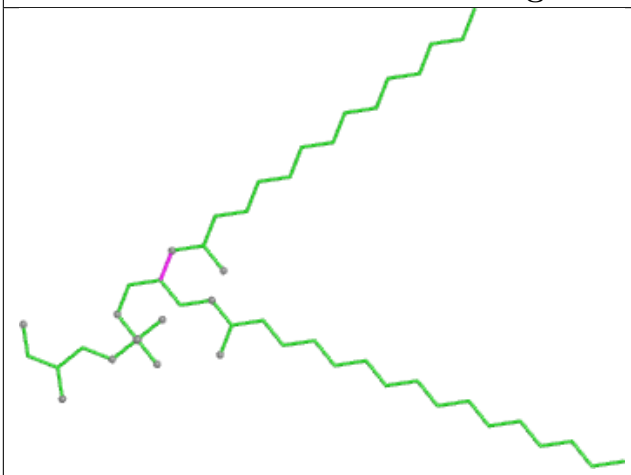


Rings

Ligand LHG 6 617



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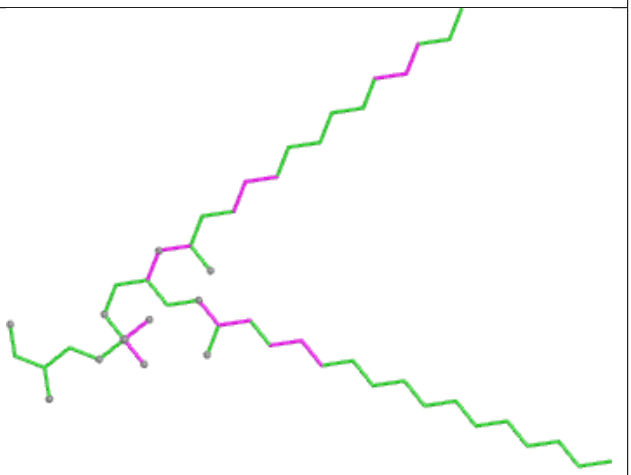
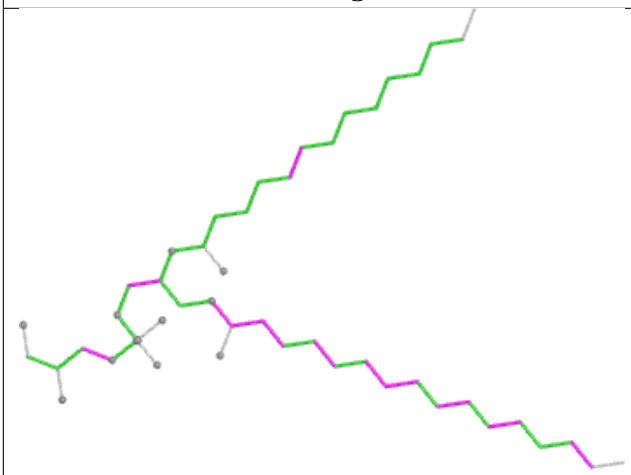
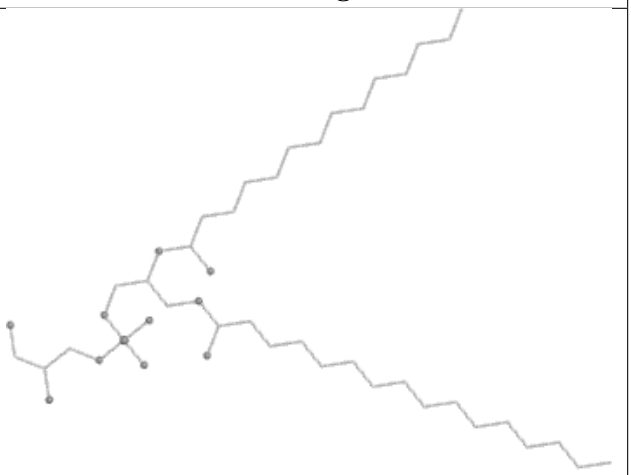


Bond angles

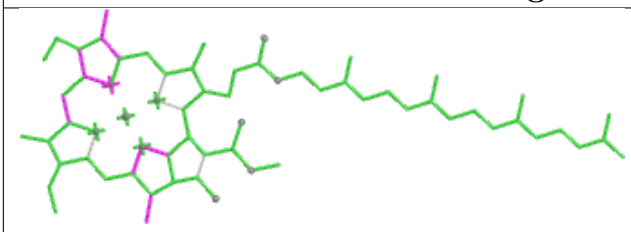


Torsions

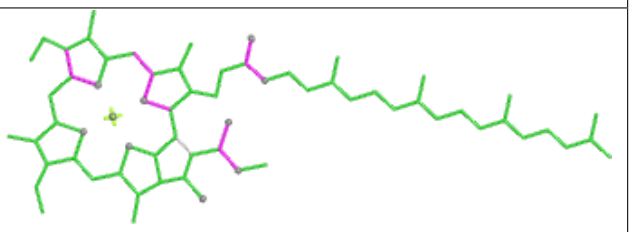


Rings

Ligand CLA d 402



Bond lengths



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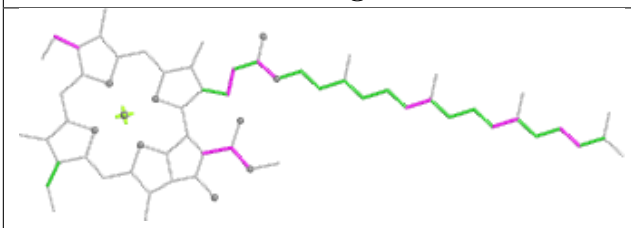

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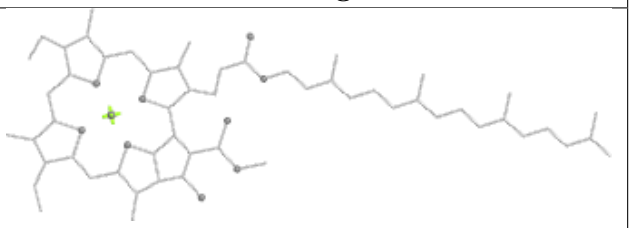
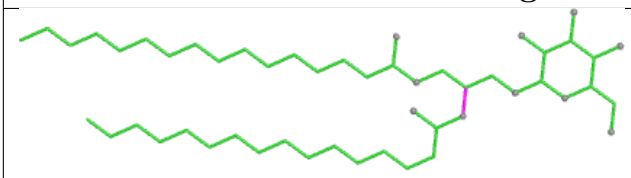
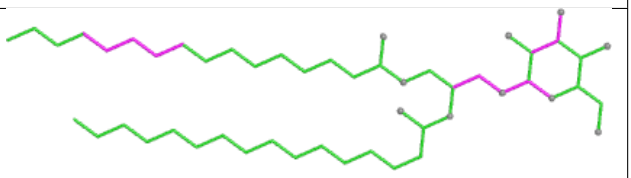


Rings

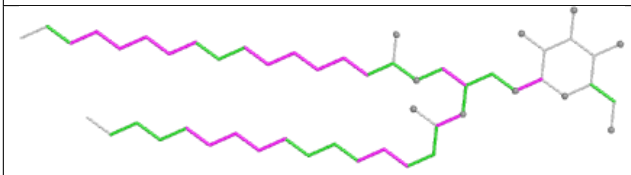
Ligand LMG C 519



Bond lengths



Bond angles



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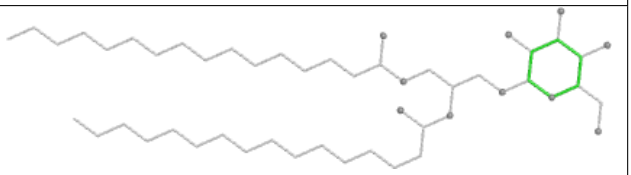
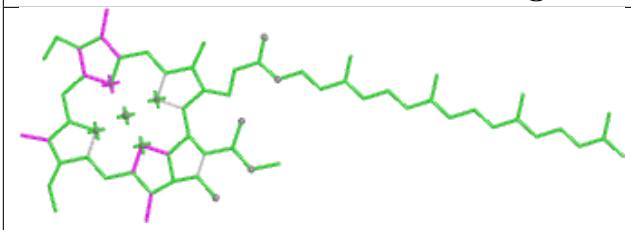


Rings

Ligand CLA v 615



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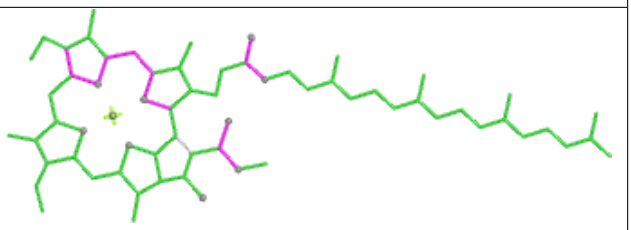
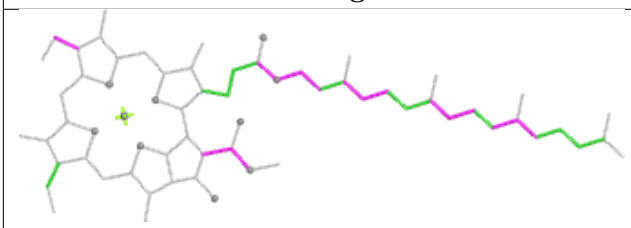


Bond angles



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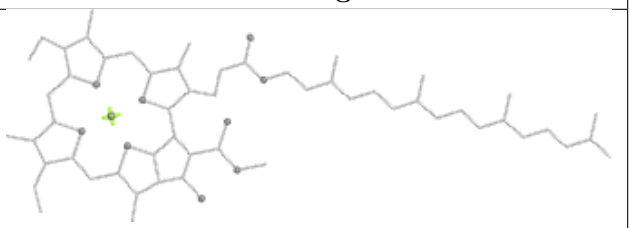
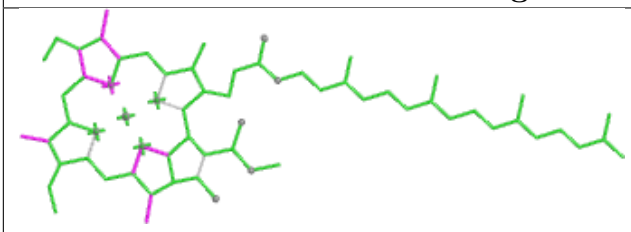
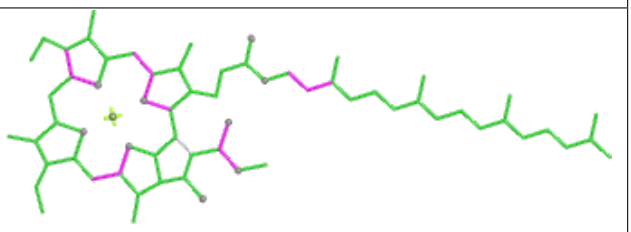
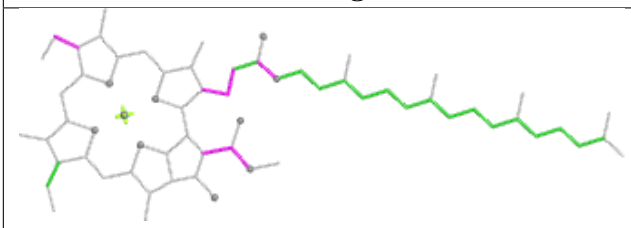
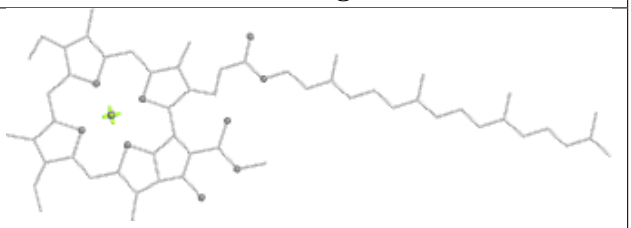


Rings

Ligand CLA BD 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

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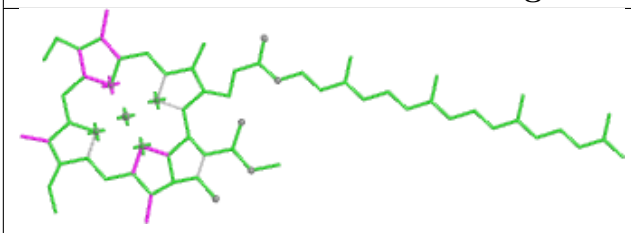
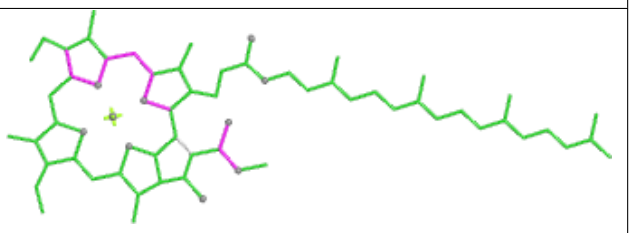
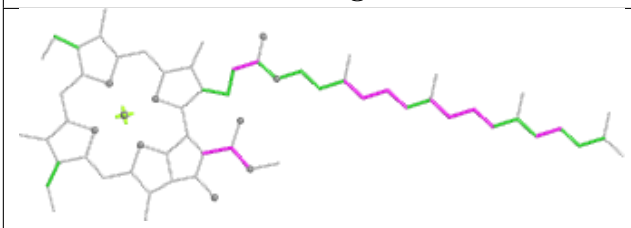
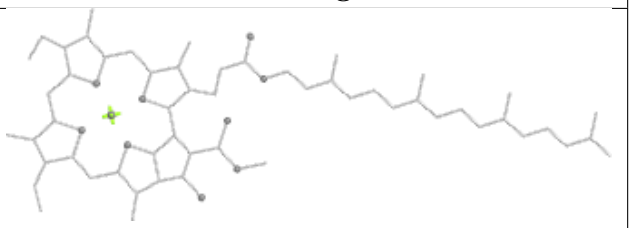
 Bond lengths	 Bond angles
 Torsions	 Rings

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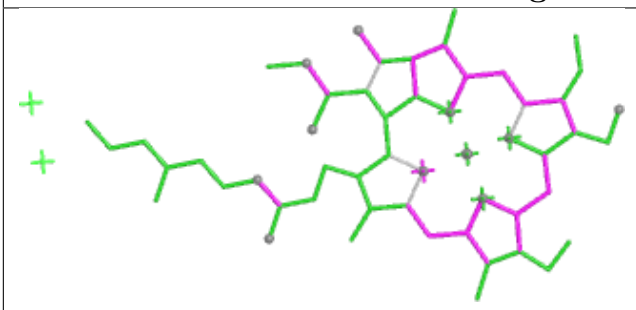
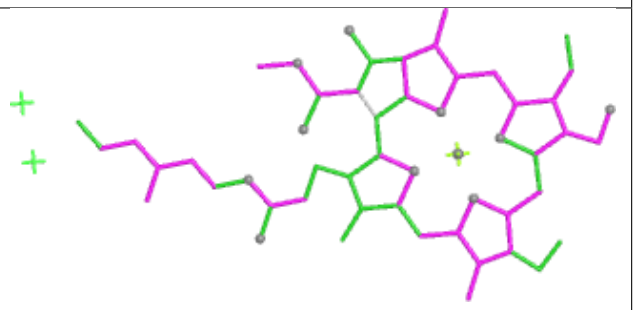
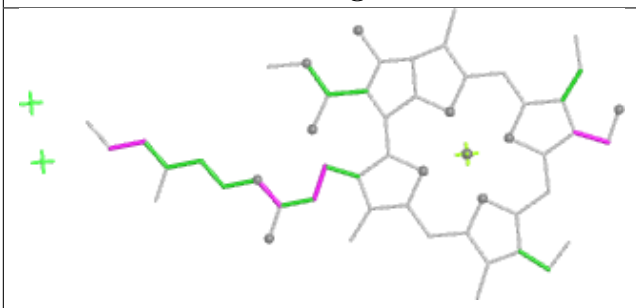
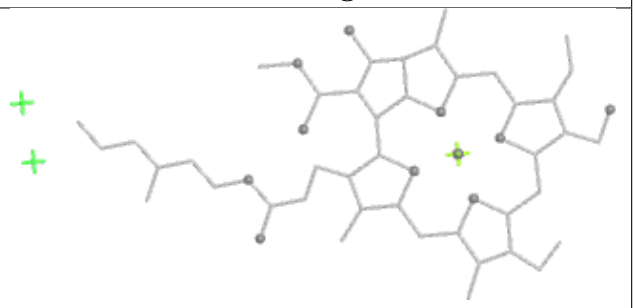
 Bond lengths	 Bond angles
 Torsions	 Rings

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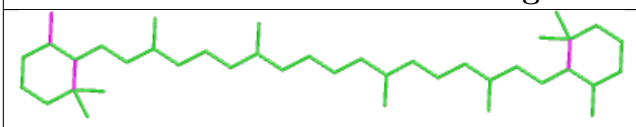
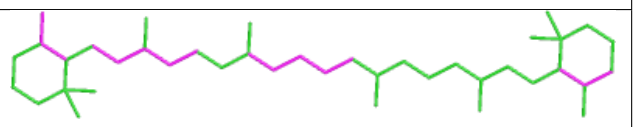
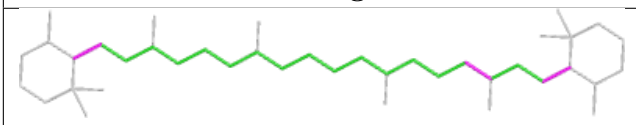
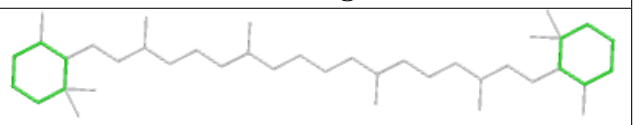
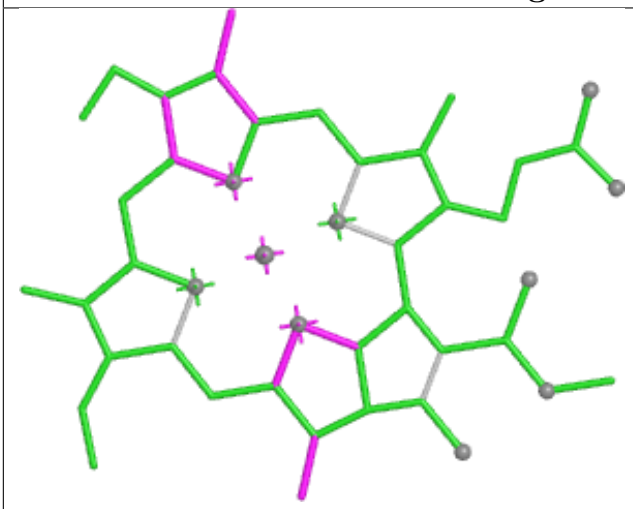
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 612



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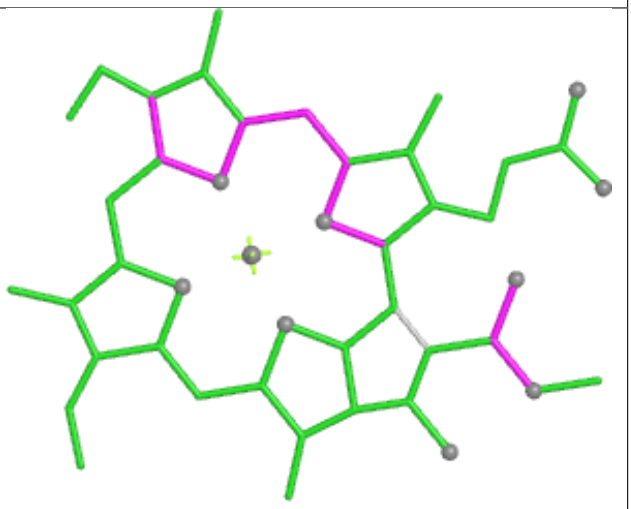
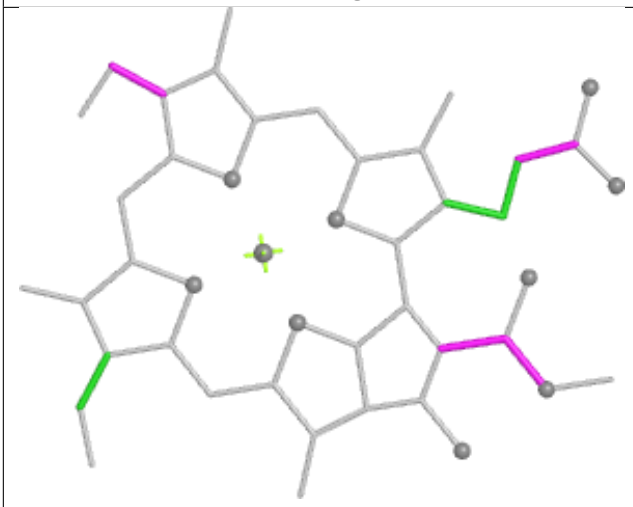


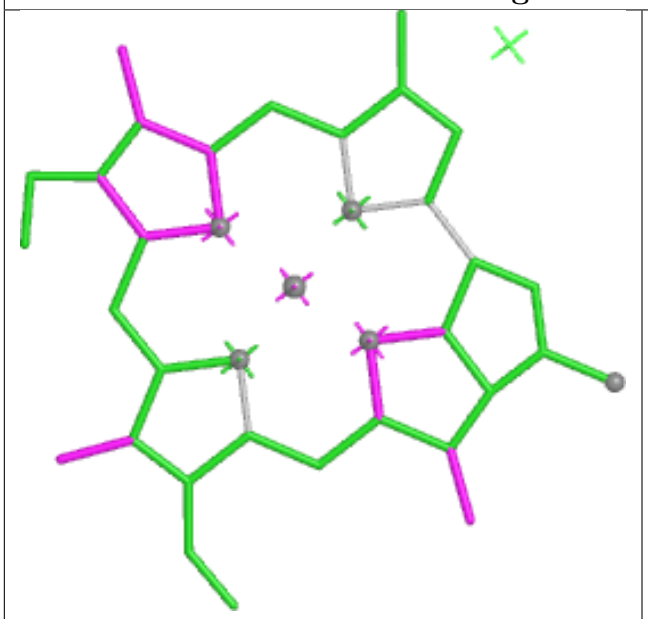
Bond angles



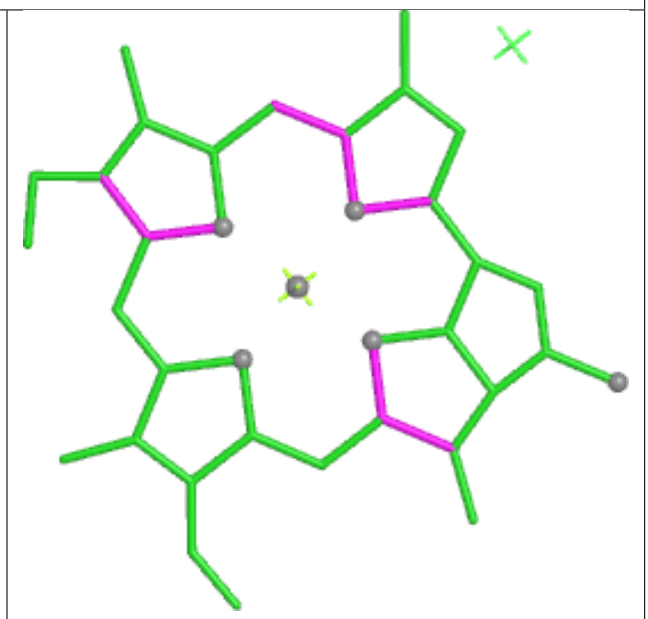
Torsions

Rings

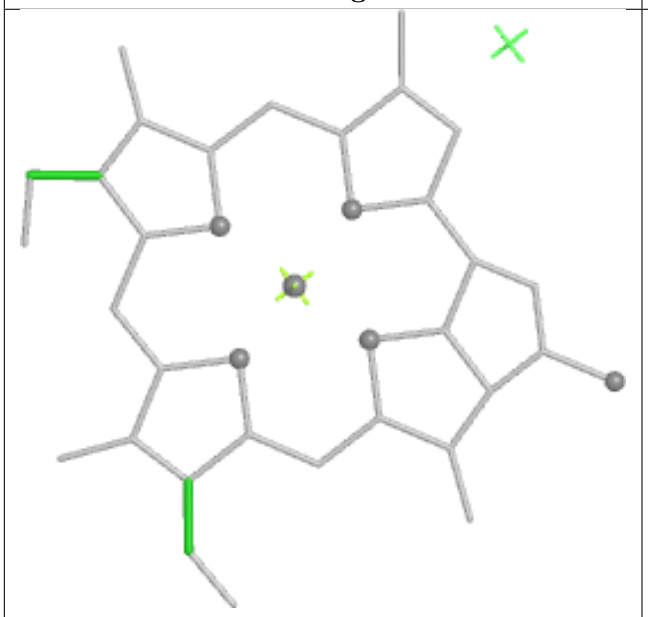
Ligand CLA BU 612



Bond lengths



Bond angles



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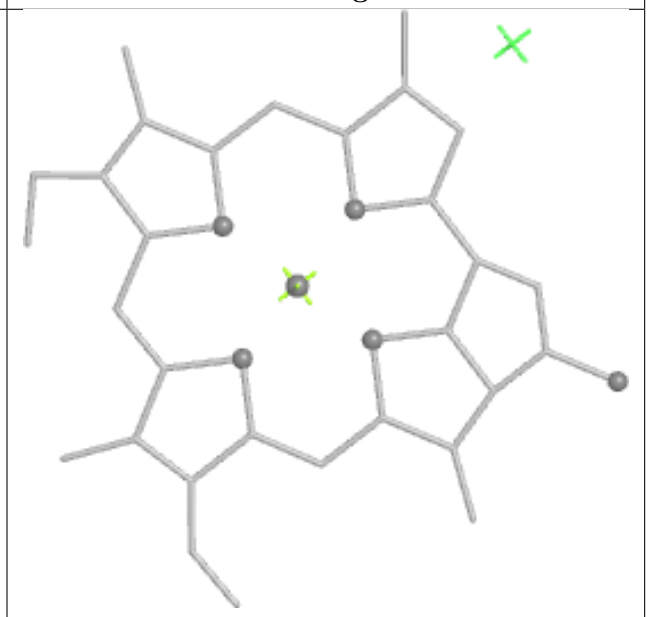
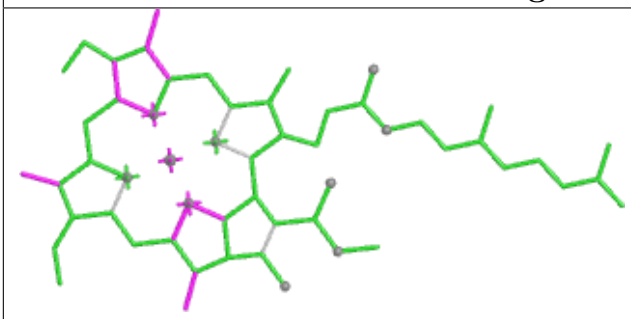


Rings

Ligand CLA 0 611



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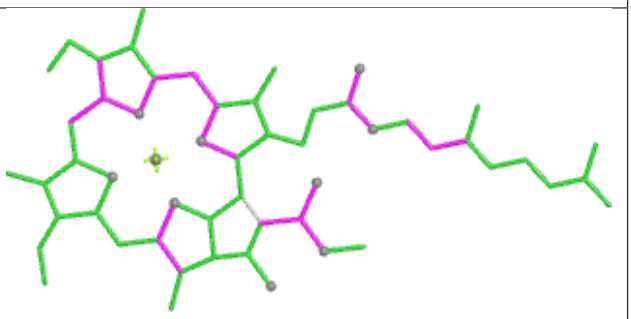

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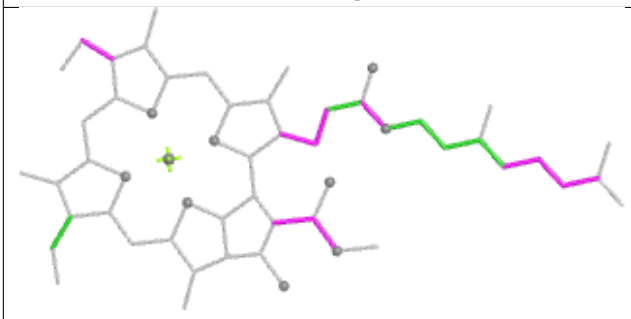

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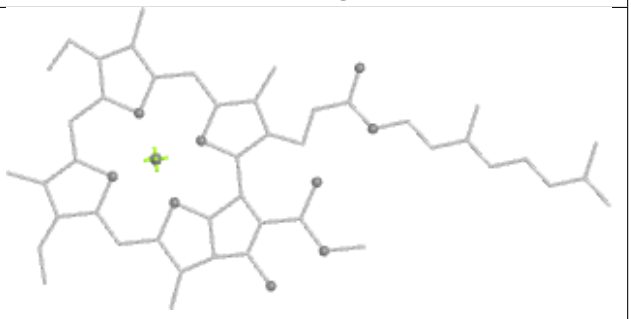
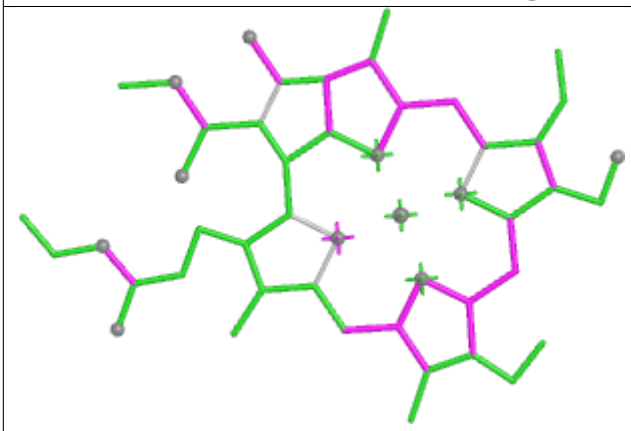


Rings

Ligand CHL Y 306



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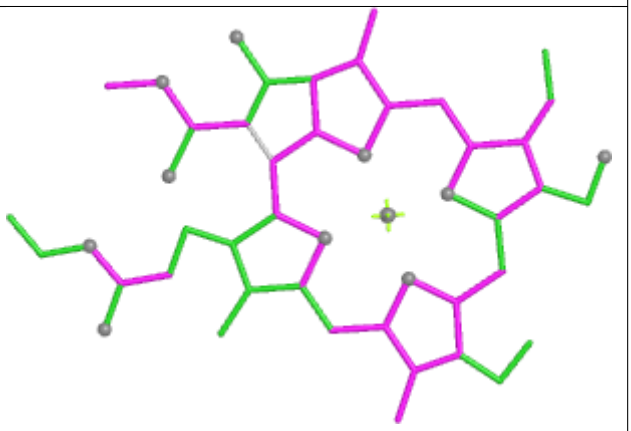
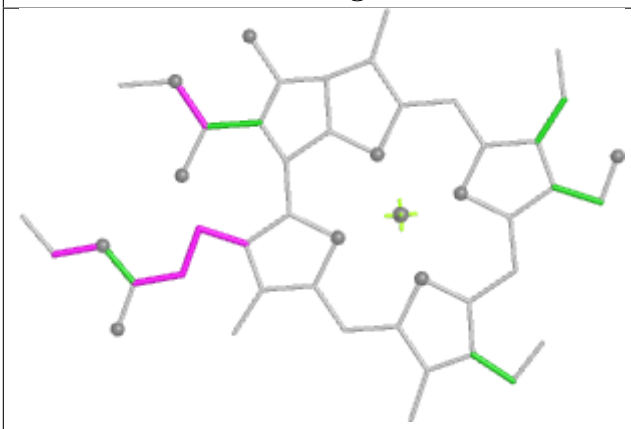
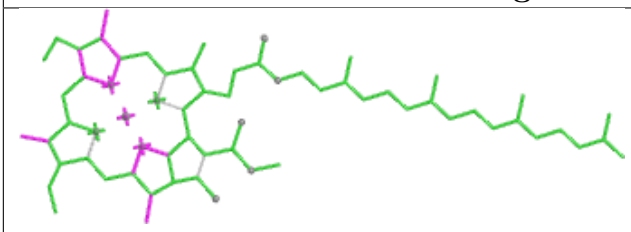
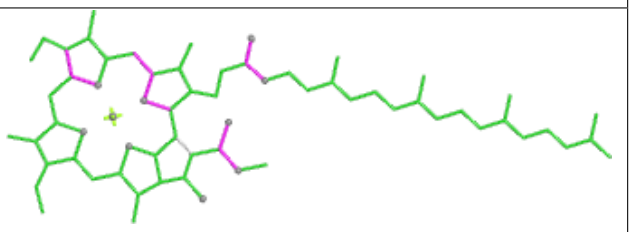
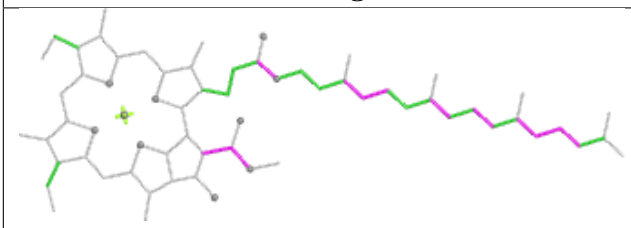
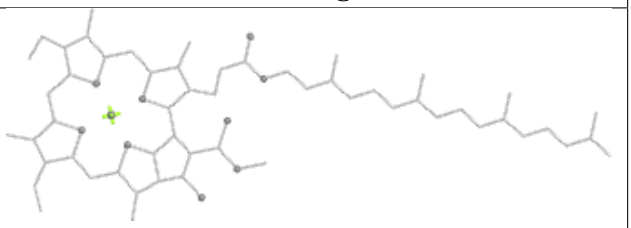


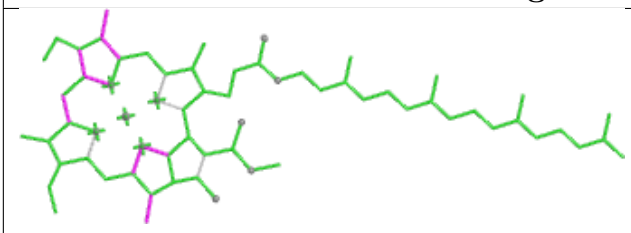
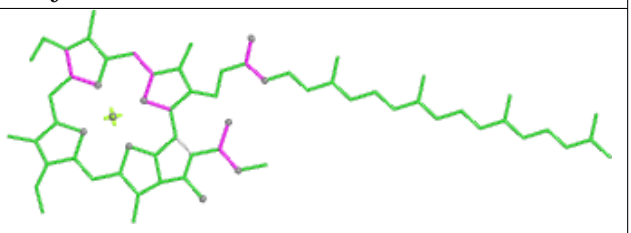
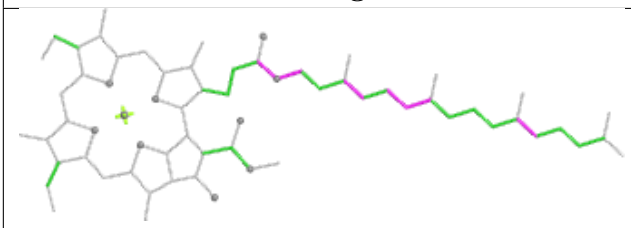
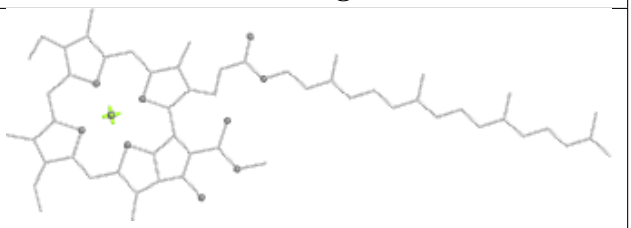
Bond angles

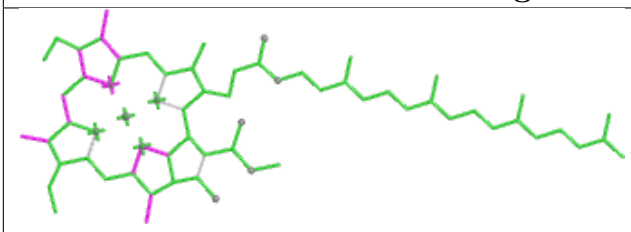
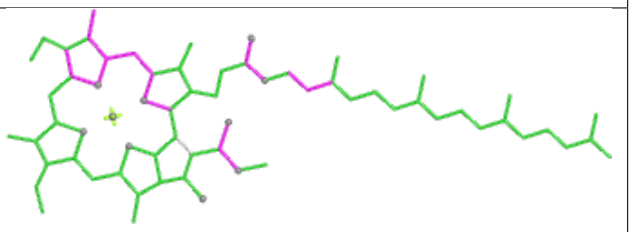
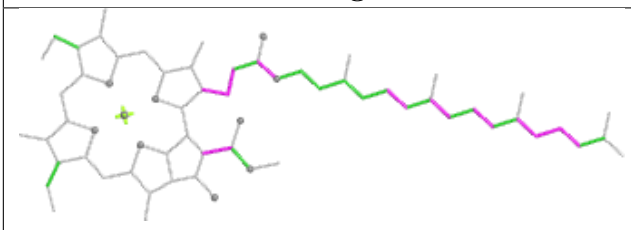
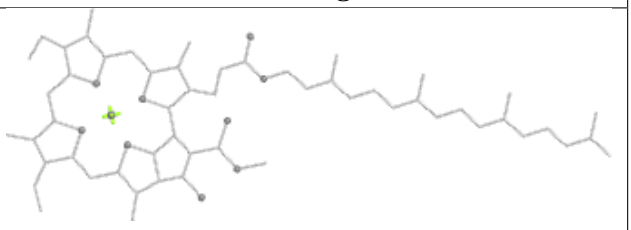


Torsions

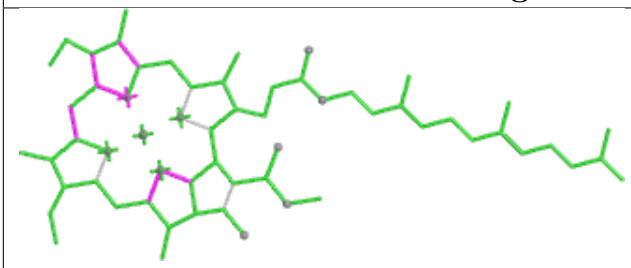
Rings

Ligand CLA BF 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

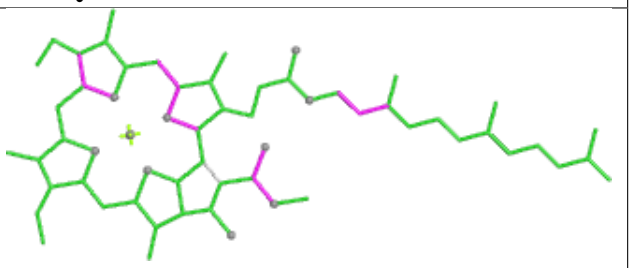
Ligand CLA y 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Au 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

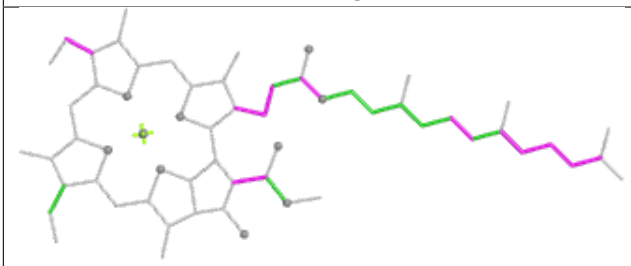
Ligand CLA BQ 611



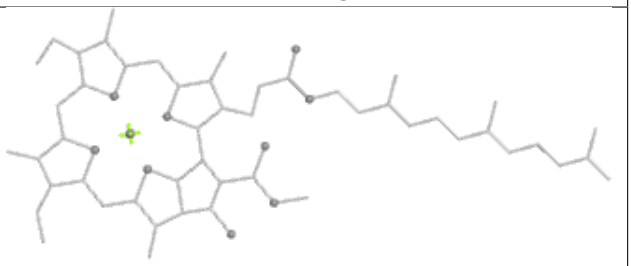
Bond lengths



Bond angles

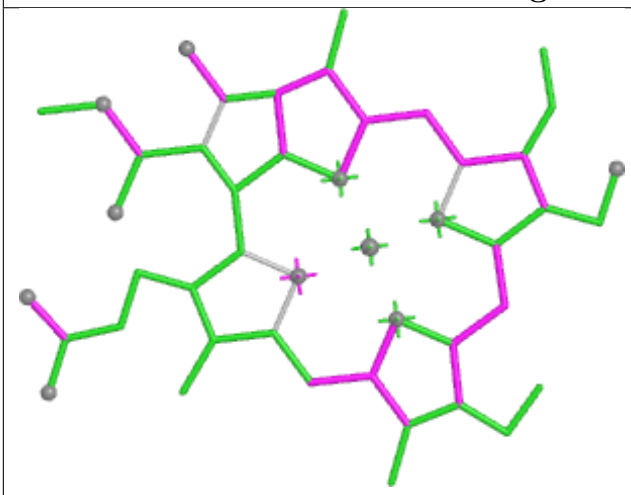


Torsions



Rings

Ligand CHL s 601



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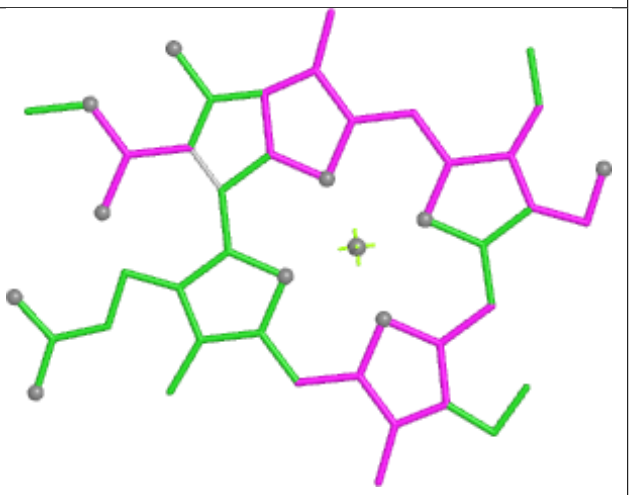

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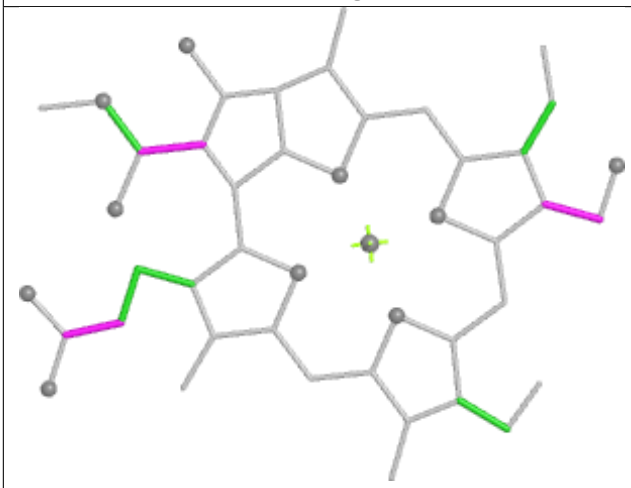

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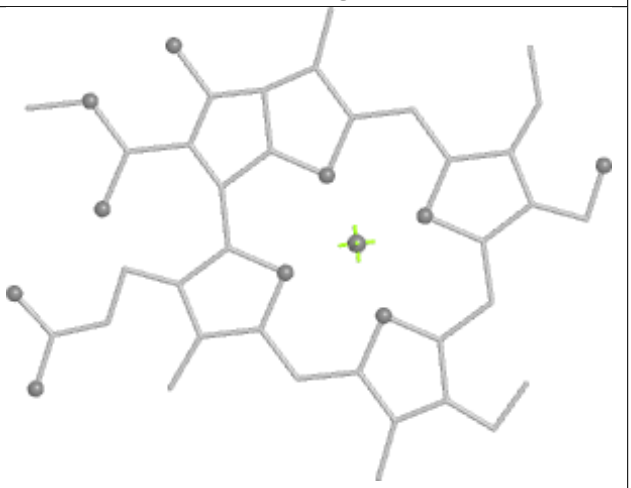
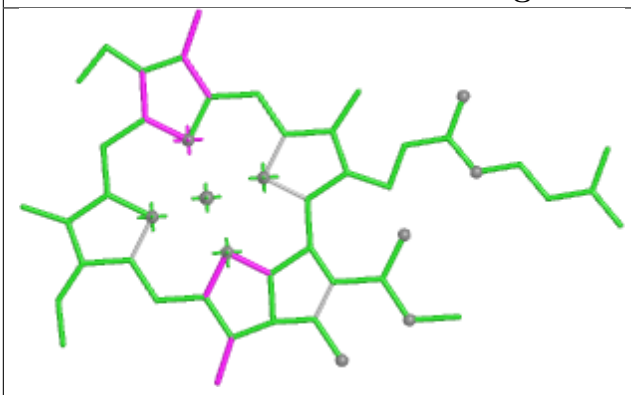
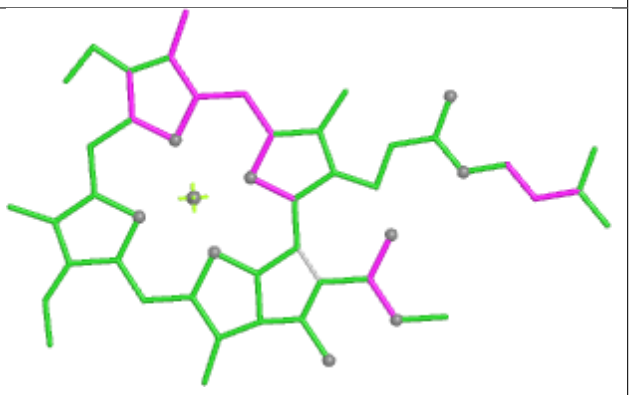
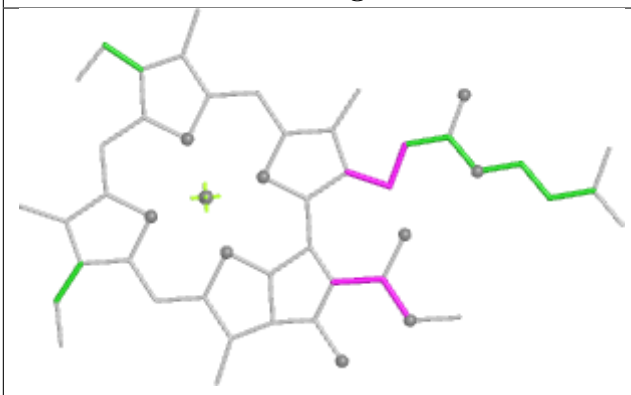
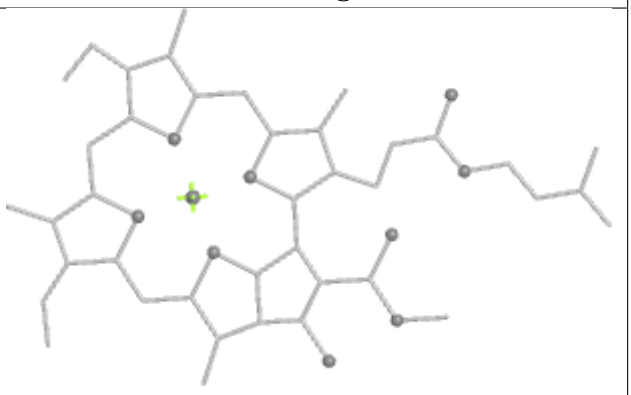


Rings

Ligand CLA Au 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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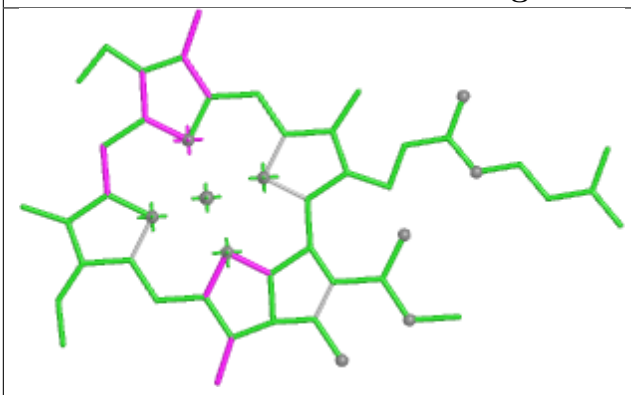
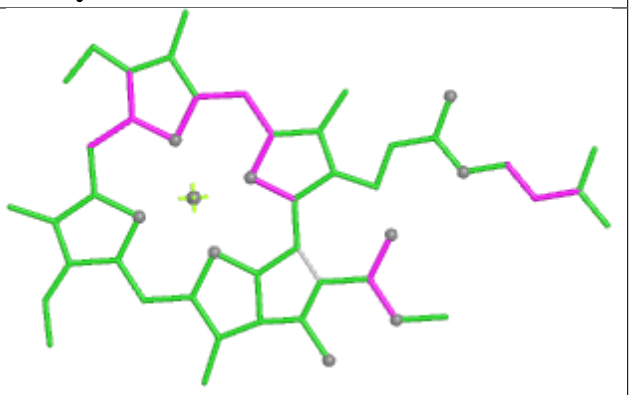
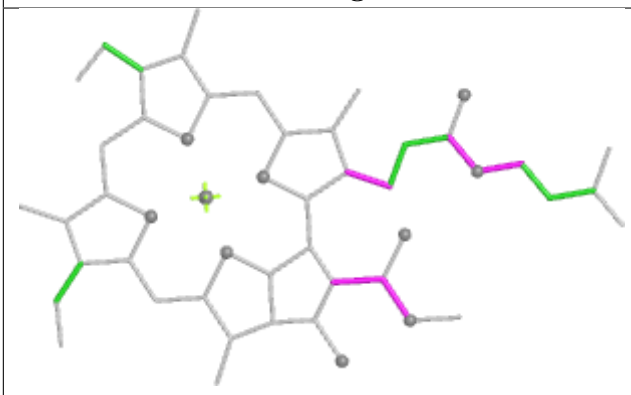
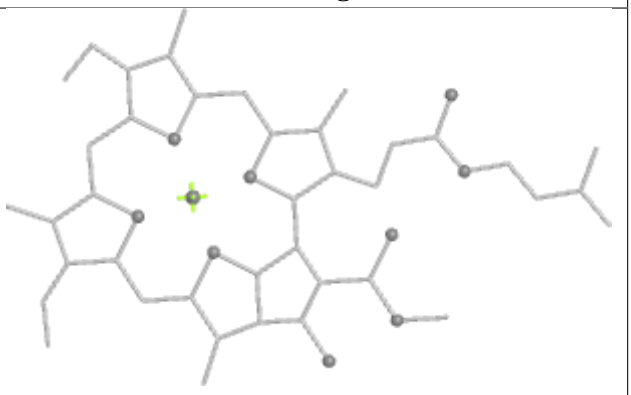
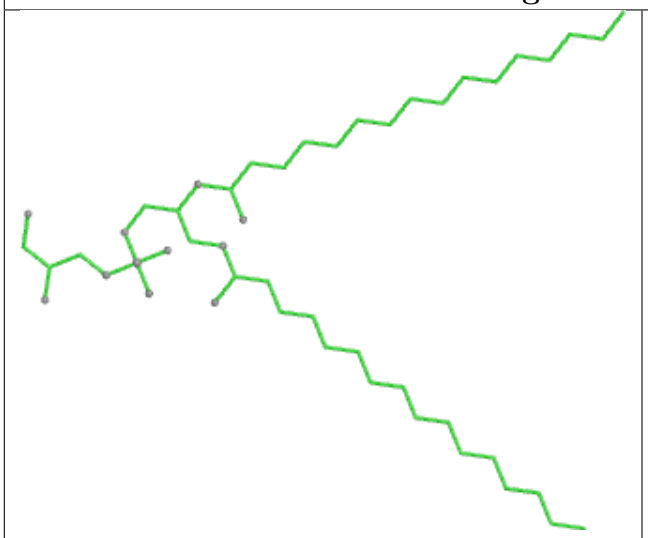
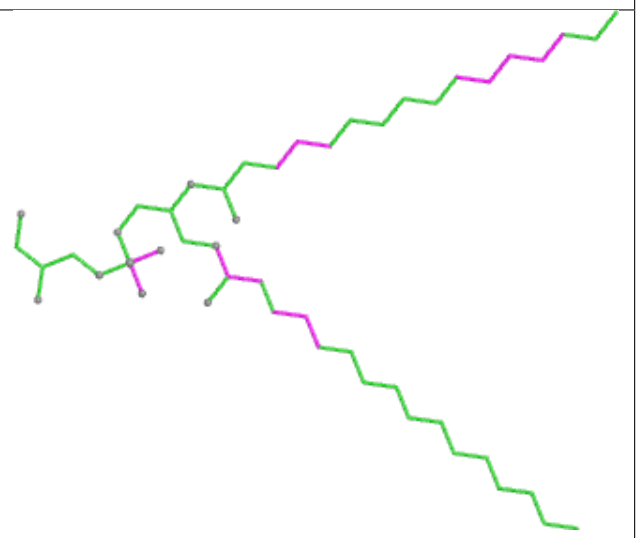
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG G 618



Bond lengths



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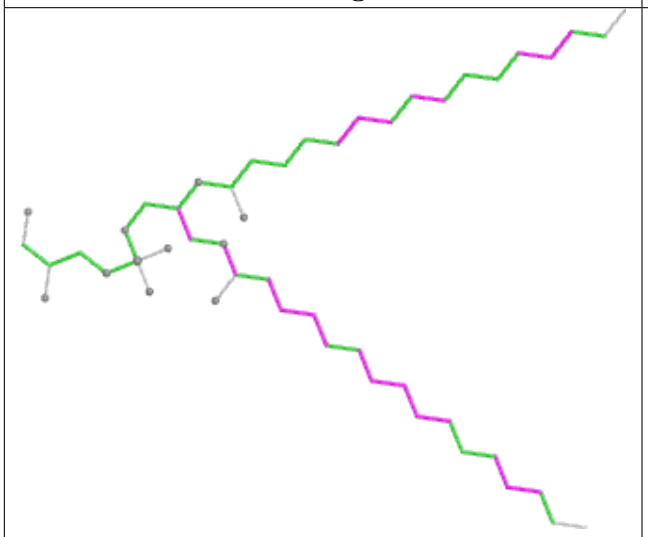

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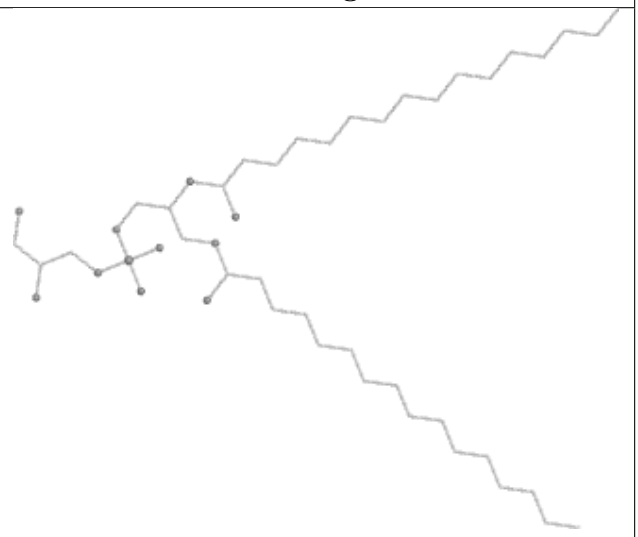
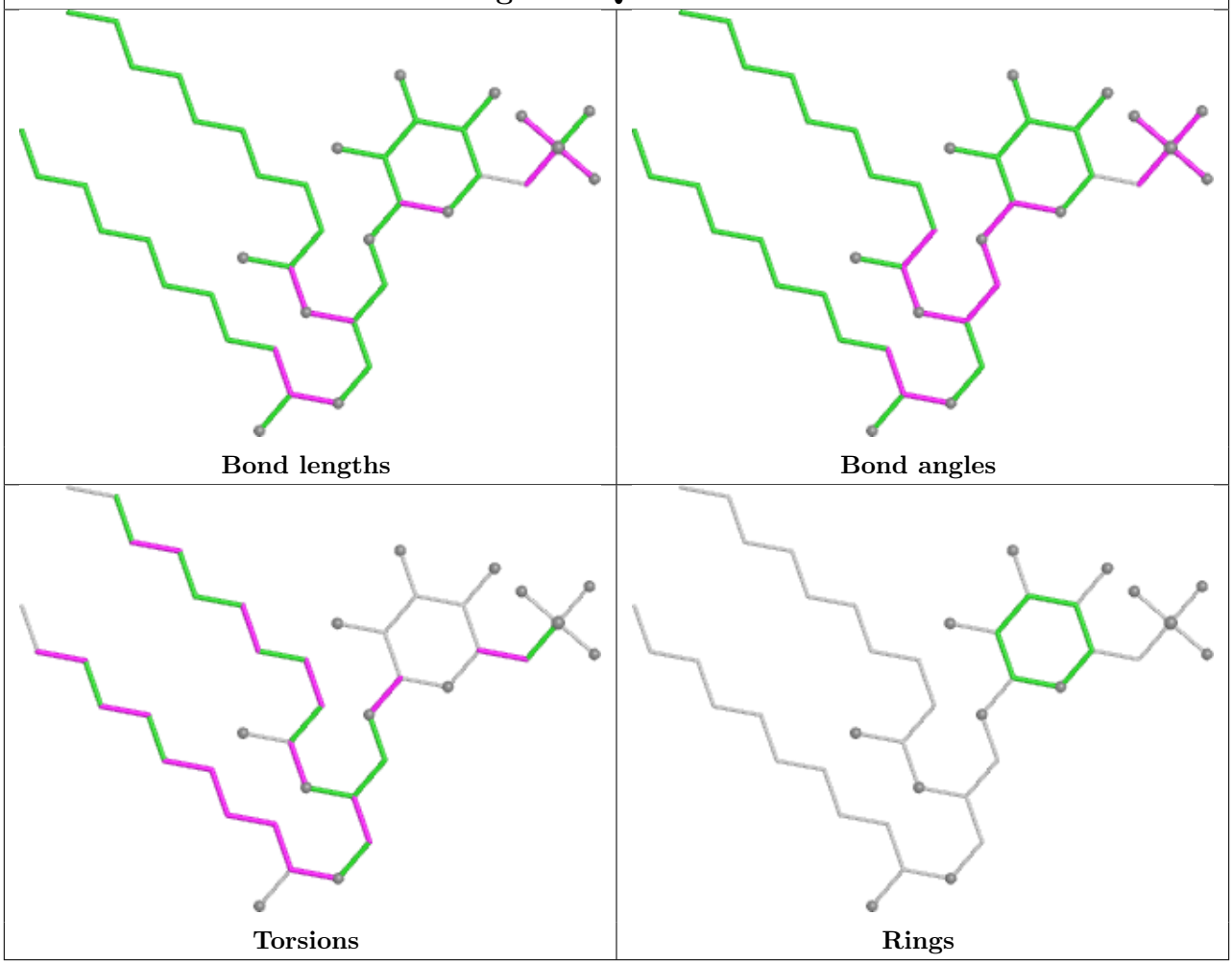
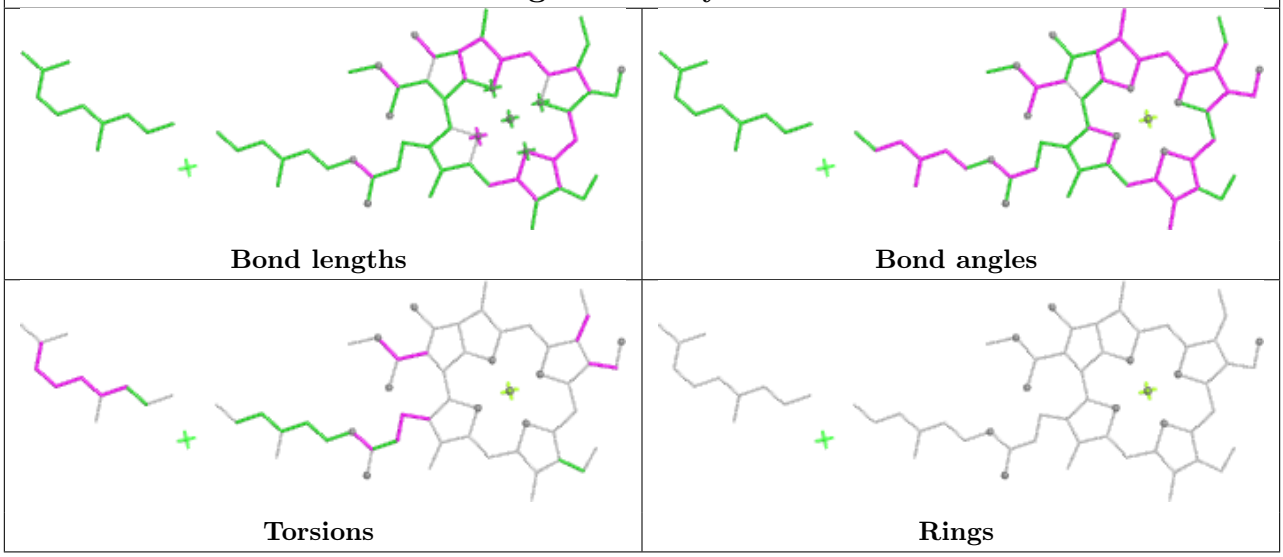


Rings

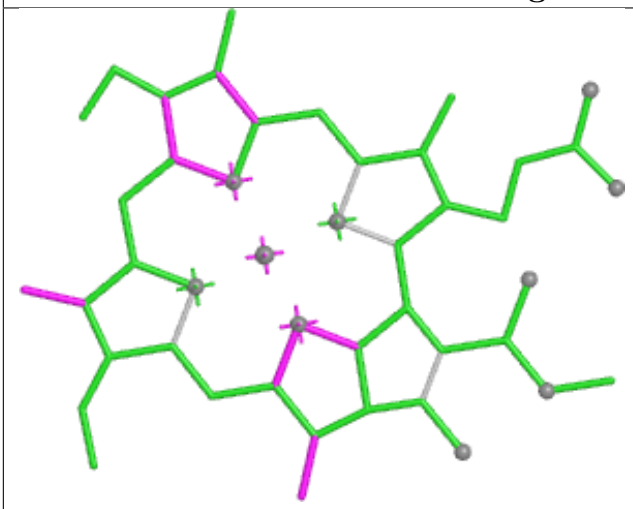
Ligand SQD Az 101



Ligand CHL y 310



Ligand CLA 8 303



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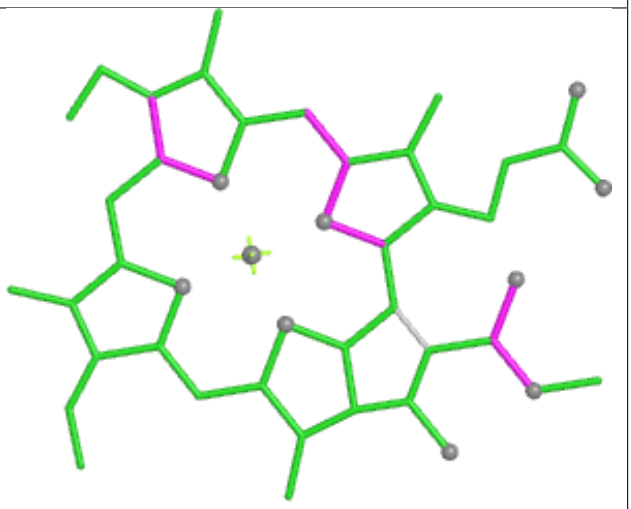

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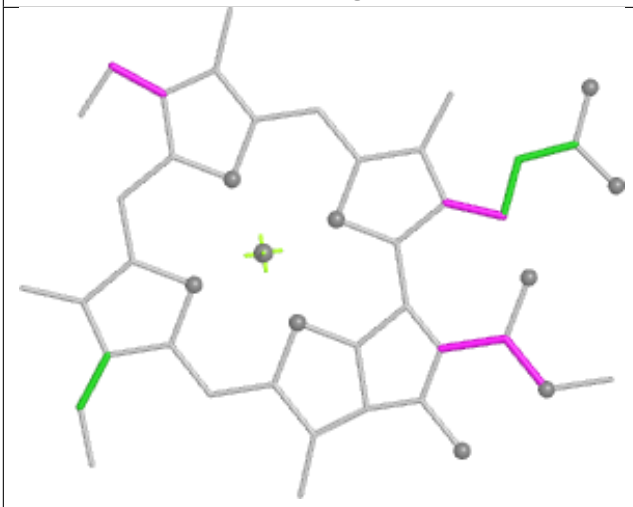
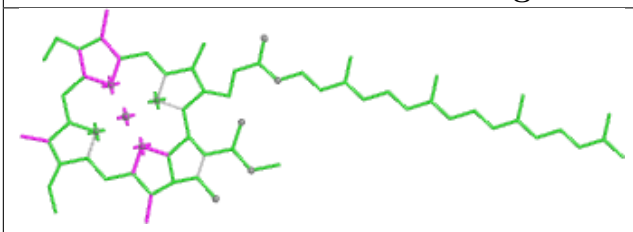


Torsions

Rings

Ligand CLA BF 513



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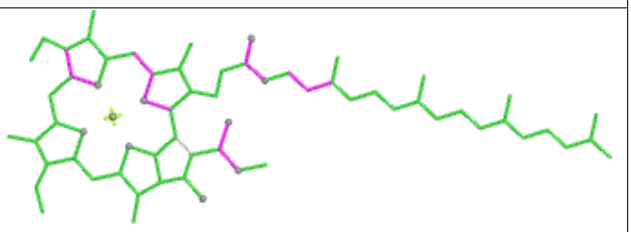

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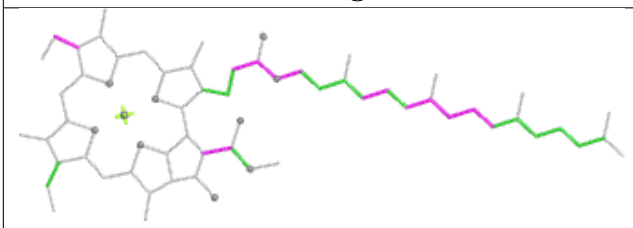

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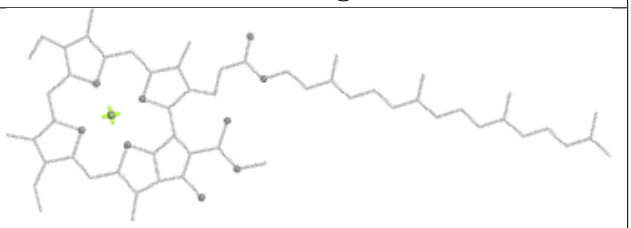
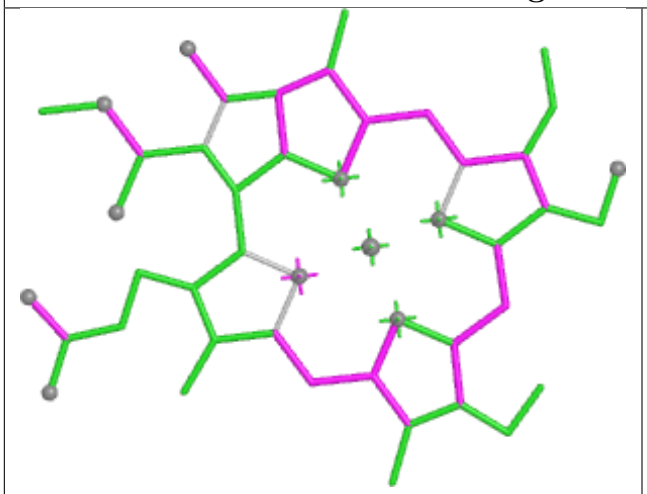


Rings

Ligand CHL S 601



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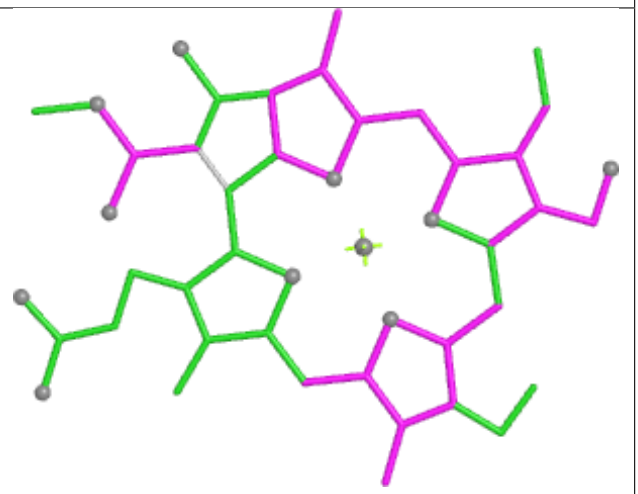
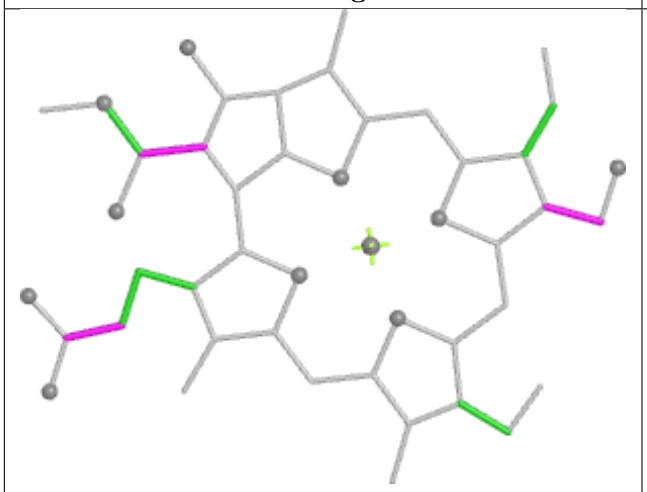


Bond angles



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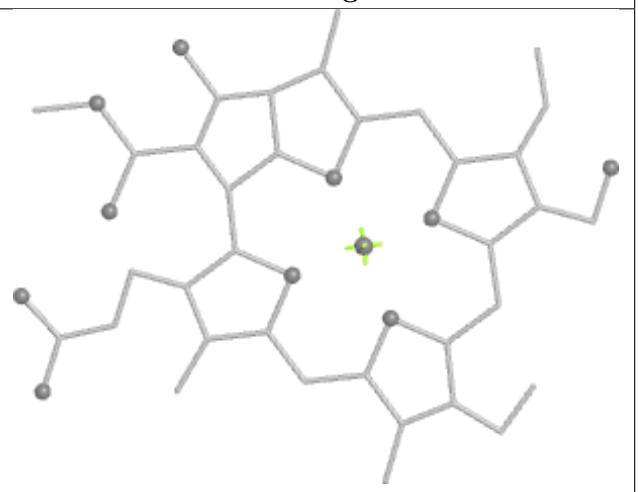
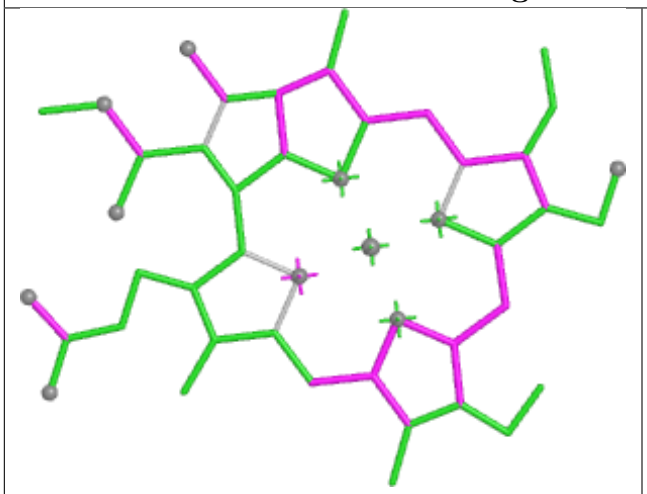


Rings

Ligand CHL BV 607



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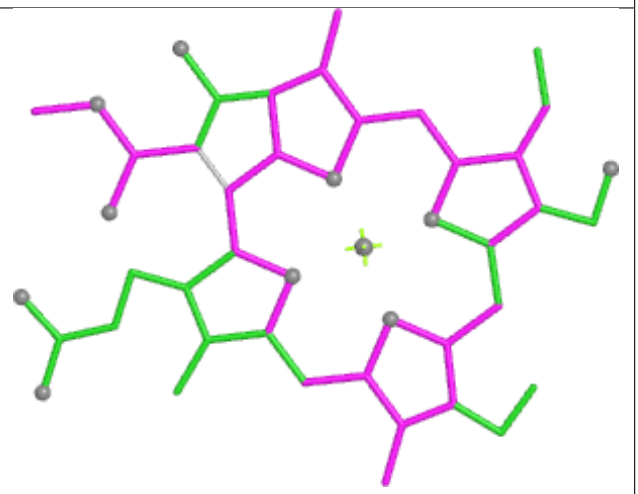
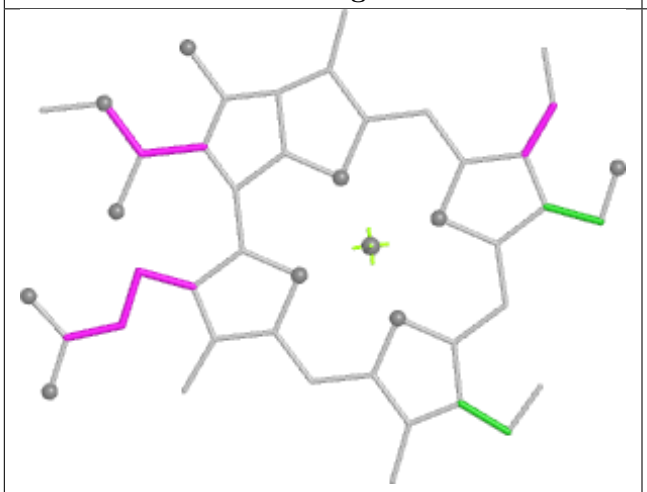
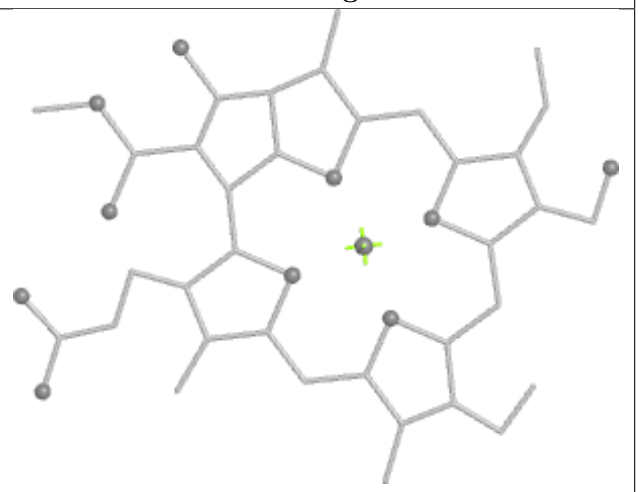


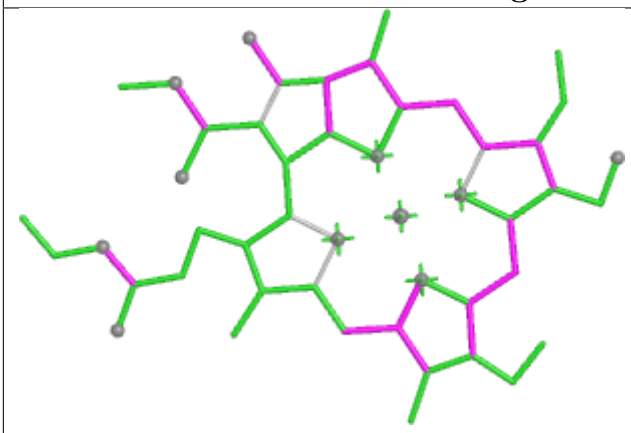
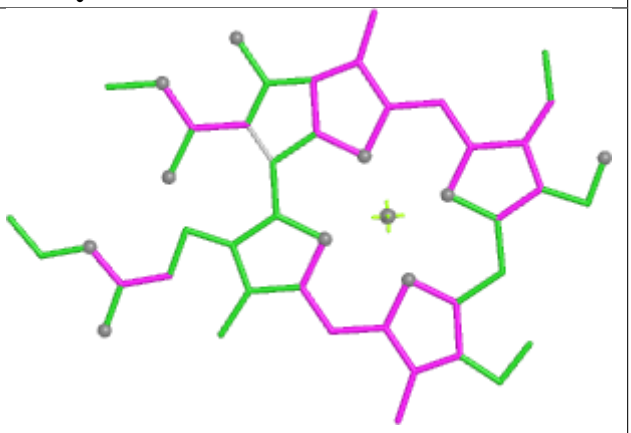
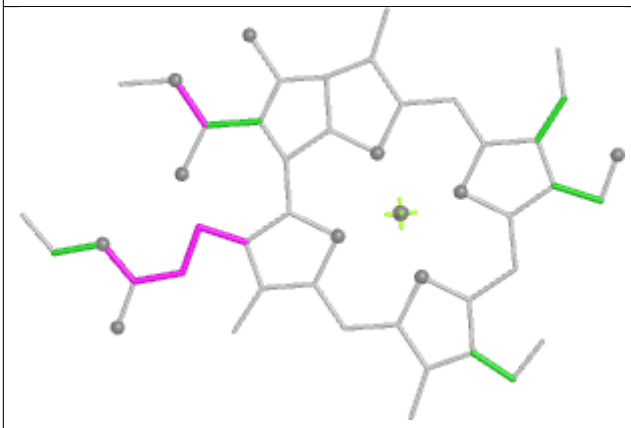
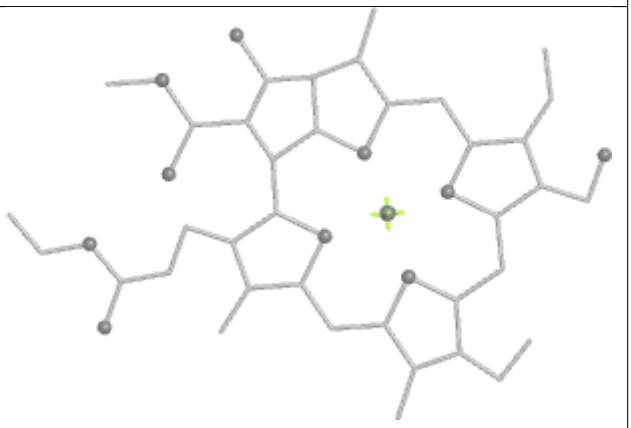
Bond angles



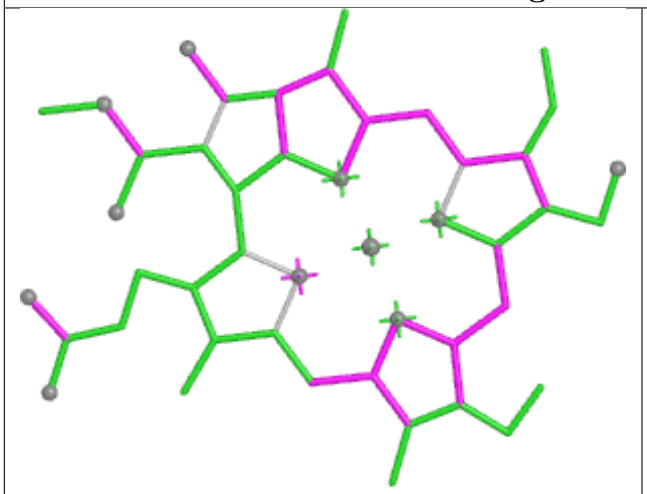
Torsions



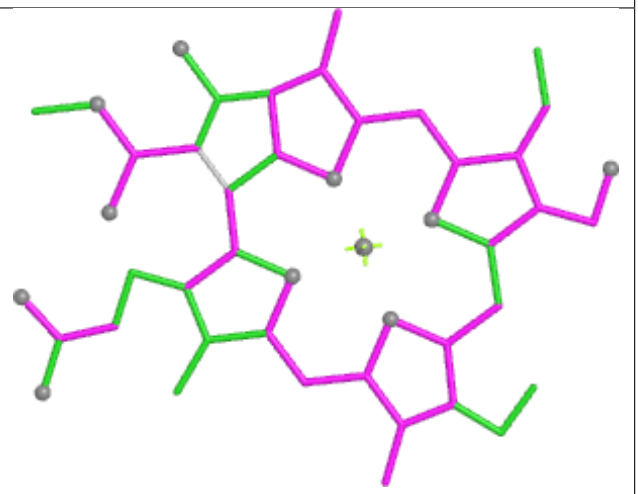
Rings

Ligand CHL BQ 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

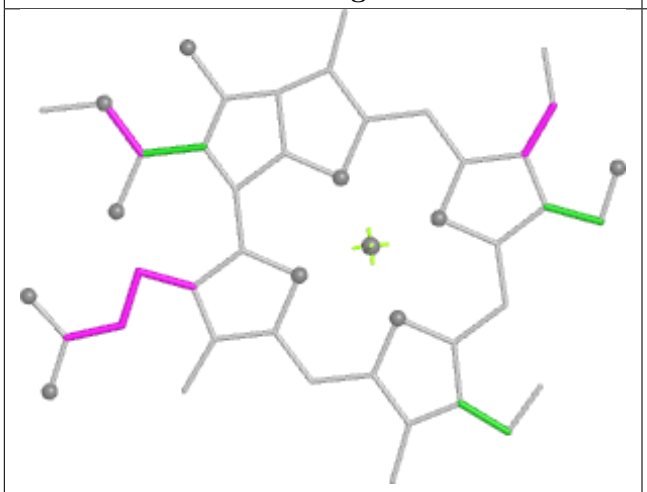
Ligand CHL 8 307



Bond lengths



Bond angles



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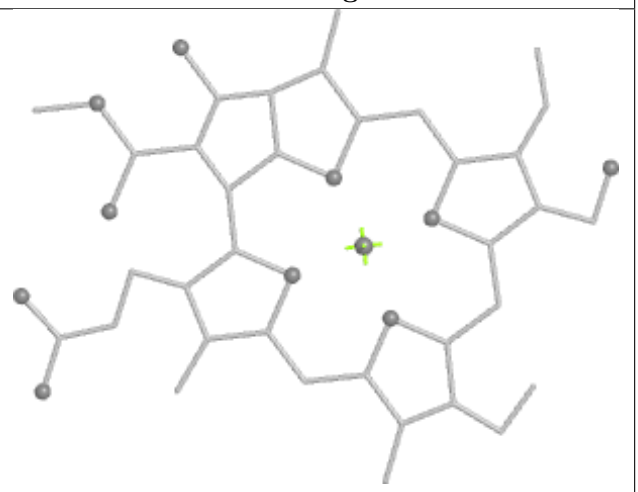
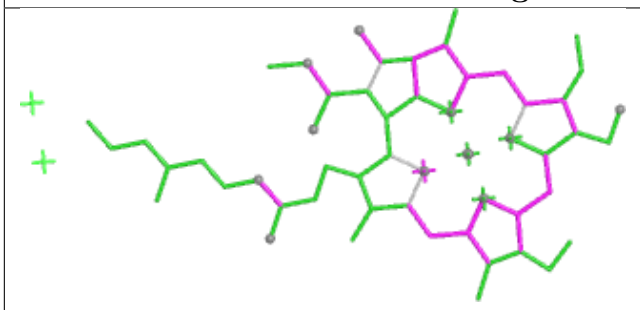
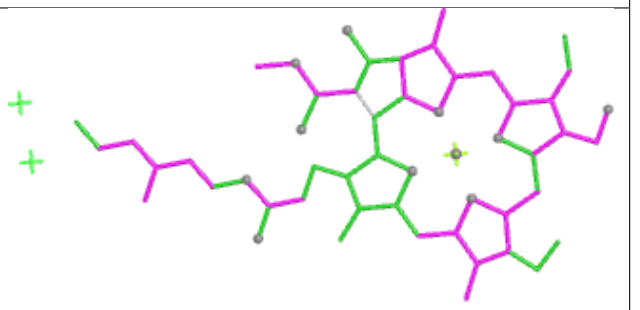
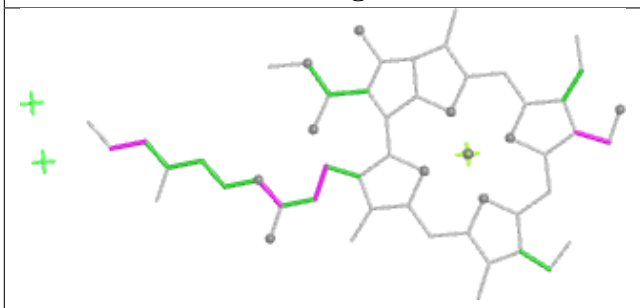
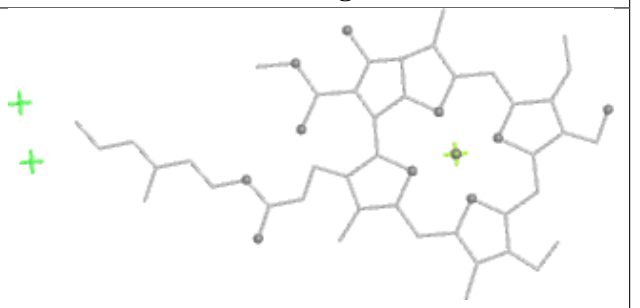
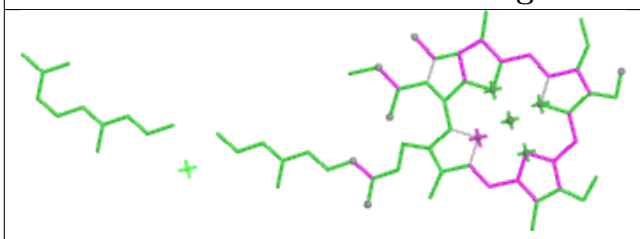
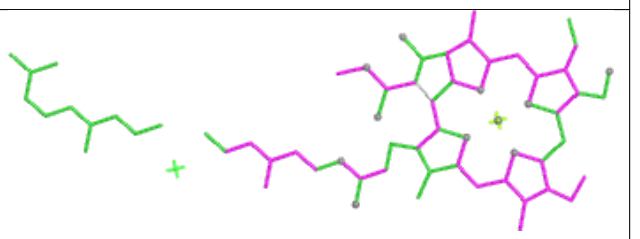
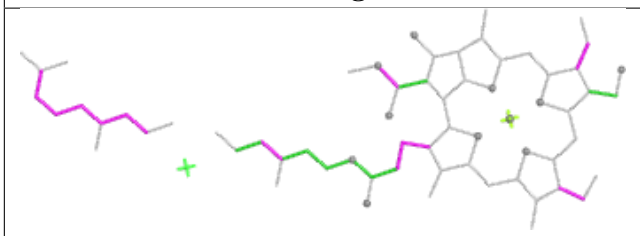
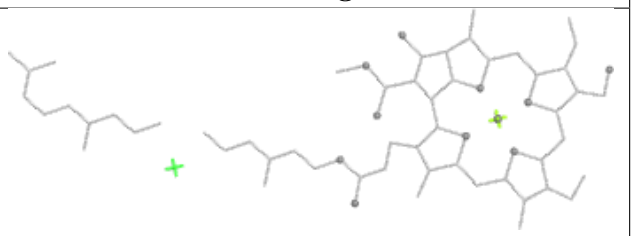
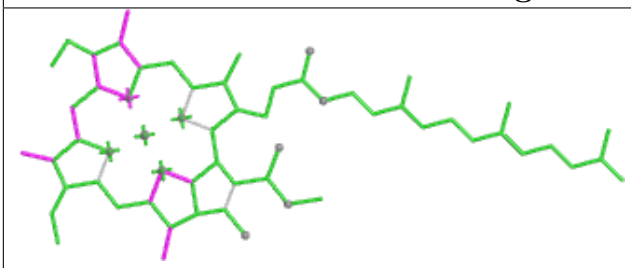


Rings

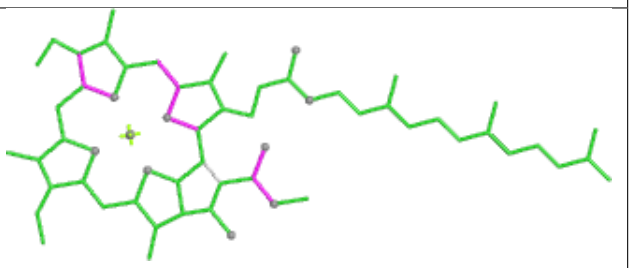
Ligand CHL BU 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Ba 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

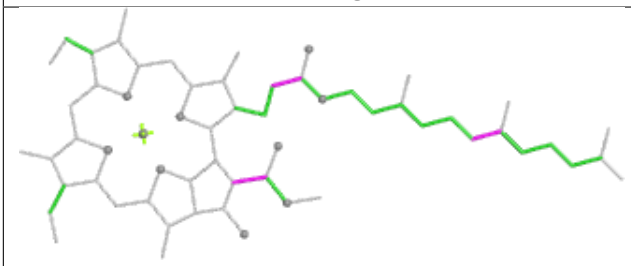
Ligand CLA A2 612



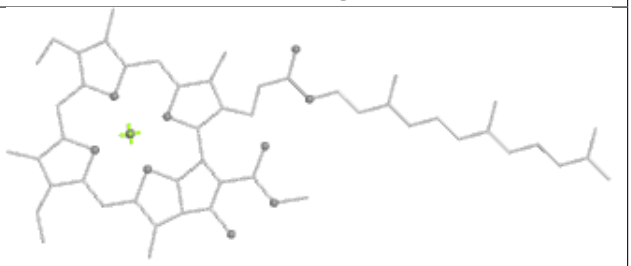
Bond lengths



Bond angles

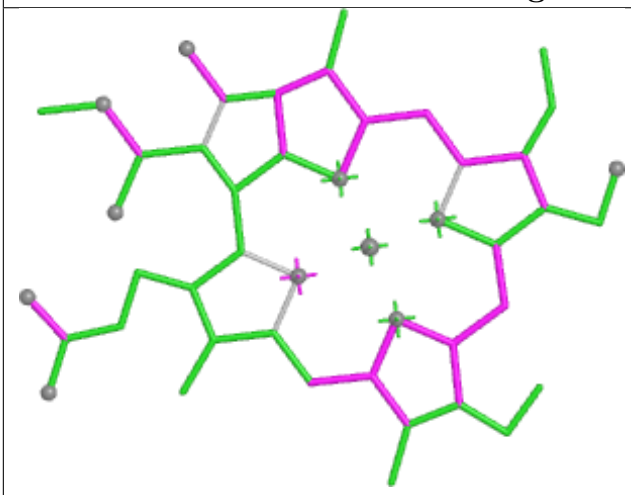


Torsions

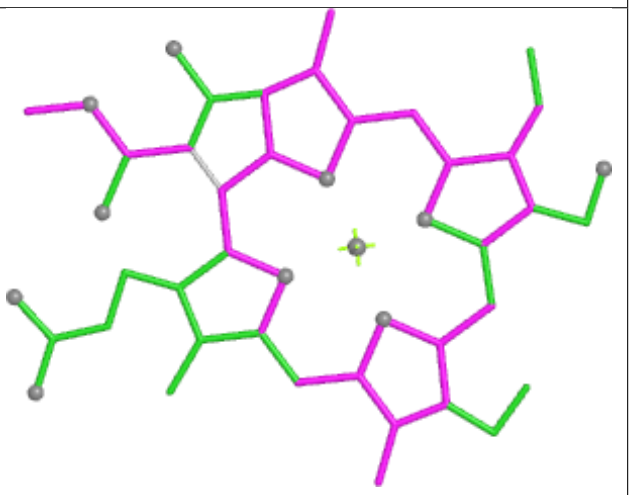


Rings

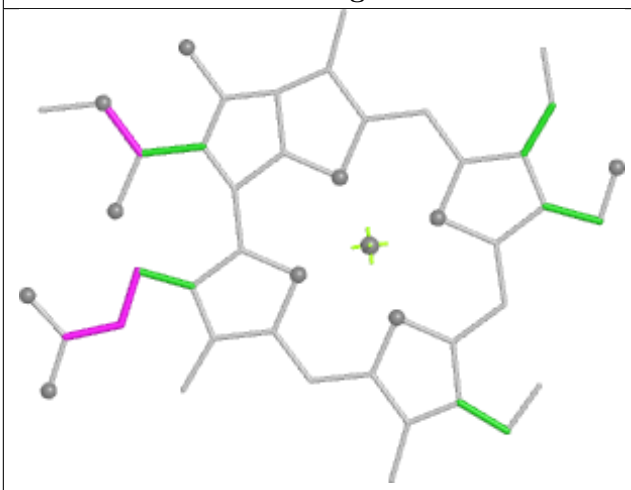
Ligand CHL 6 605



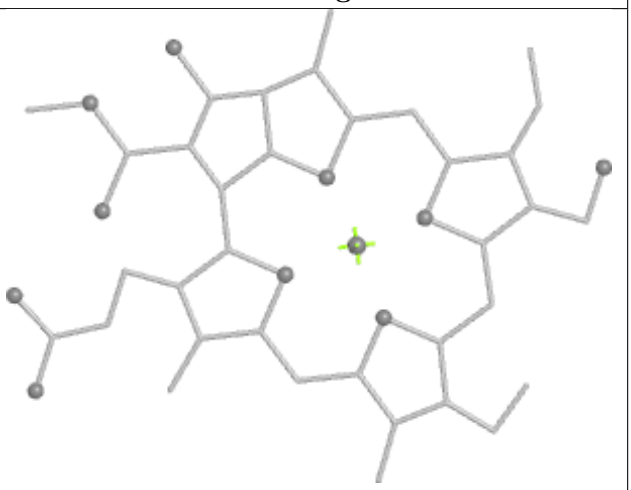
Bond lengths



Bond angles

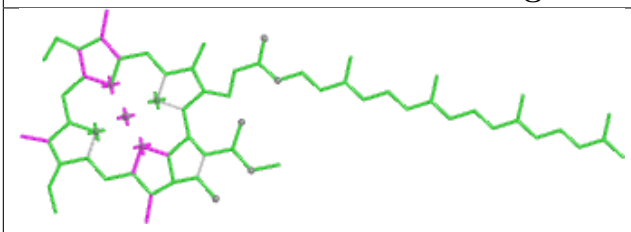


Torsions



Rings

Ligand CLA C 509



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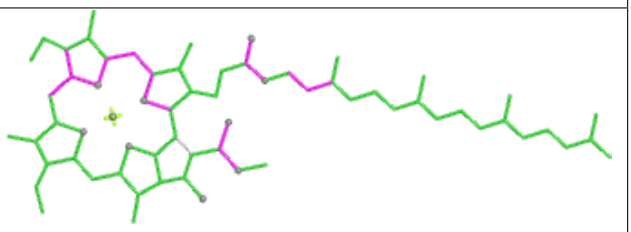
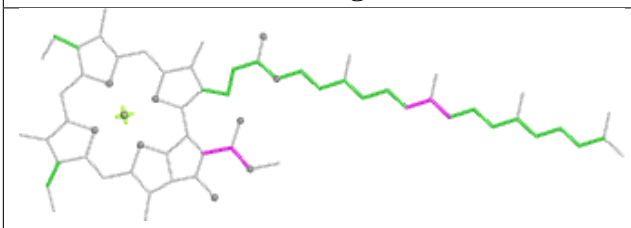


Bond angles



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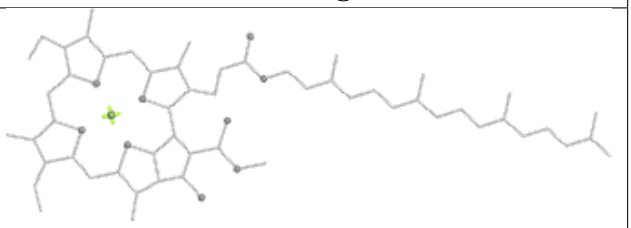
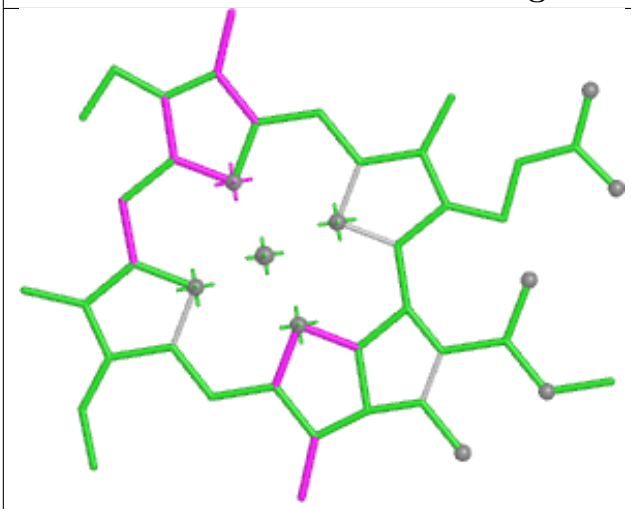


Rings

Ligand CLA 7 312



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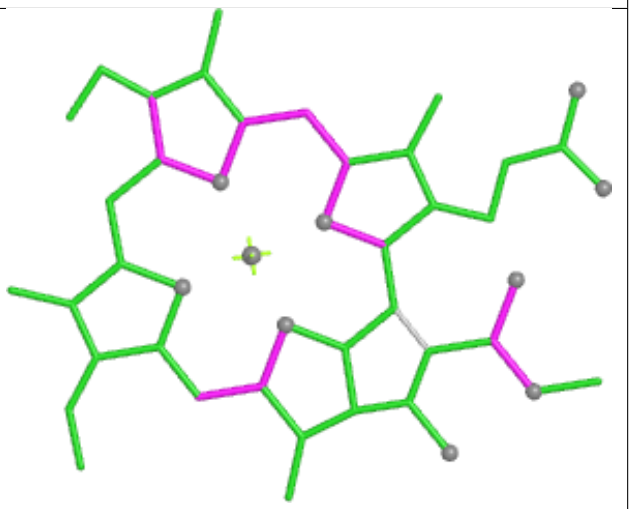
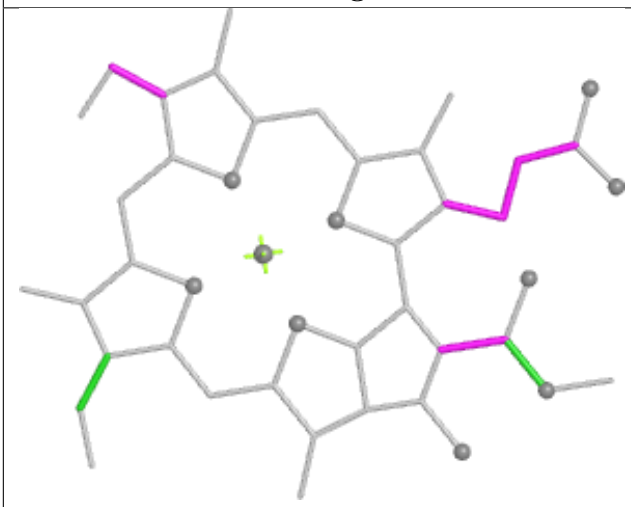


Bond angles



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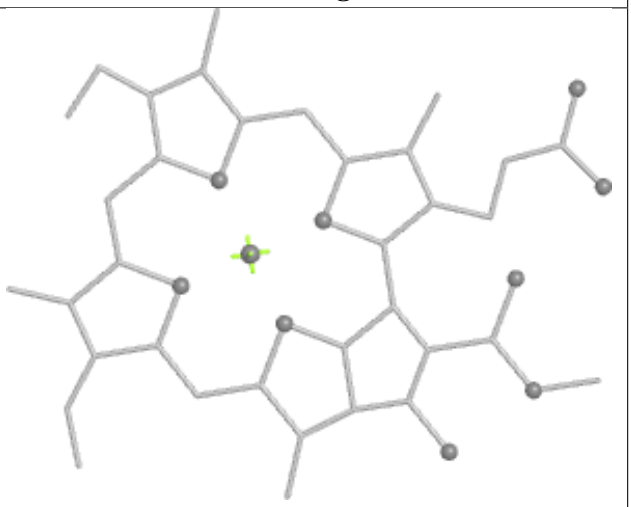
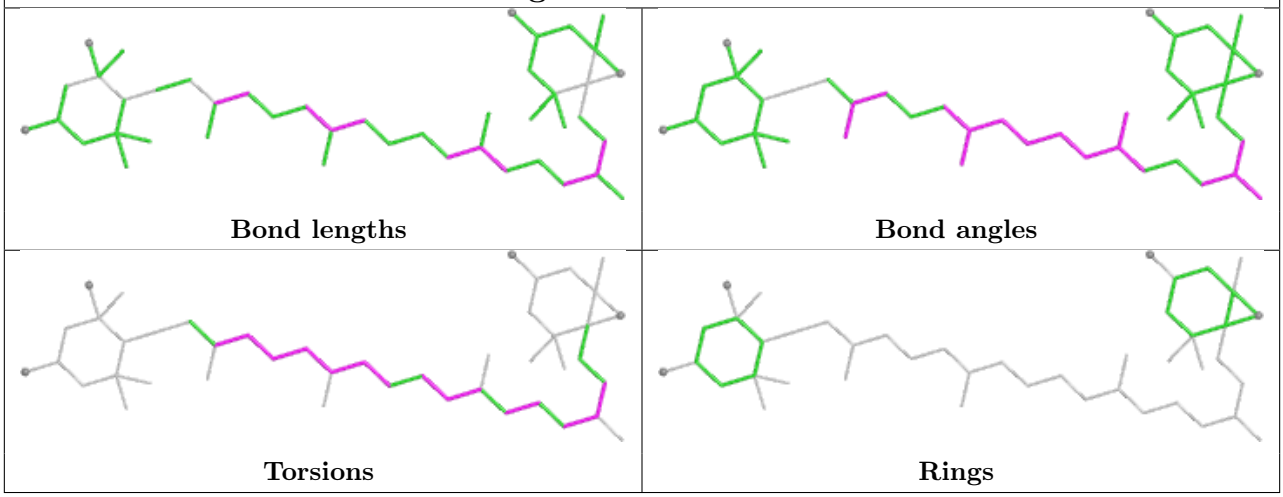
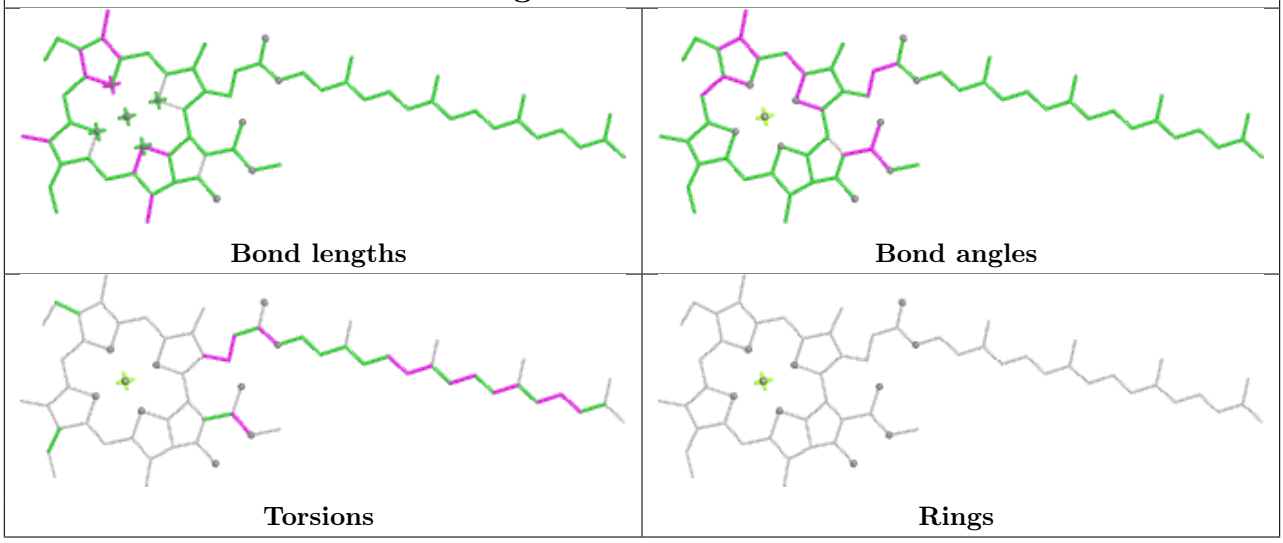


Rings

Ligand NEX r 617



Ligand CLA BE 609



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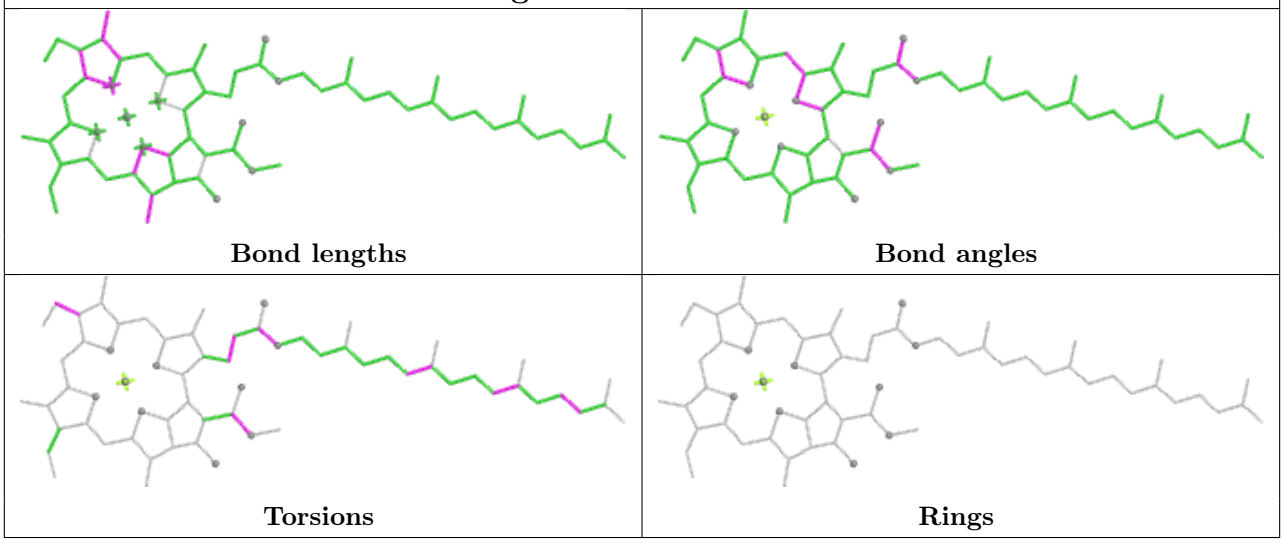

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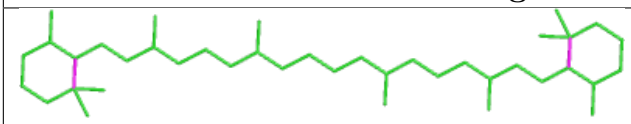
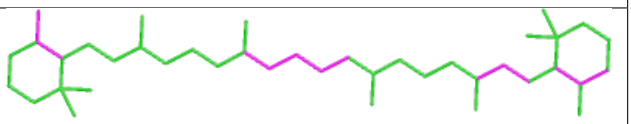
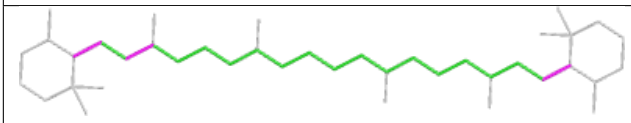


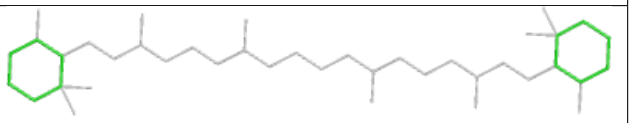
Bond lengths



Bond angles

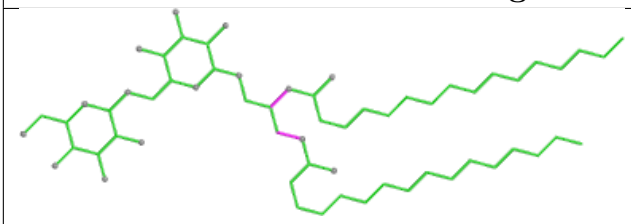


Torsions



Rings

Ligand DGD BF 518



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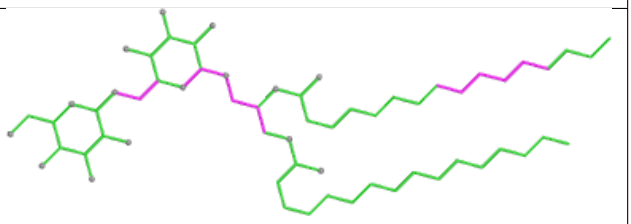
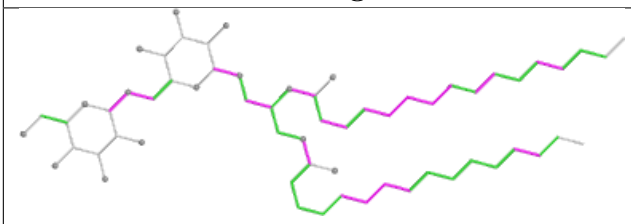


Bond angles



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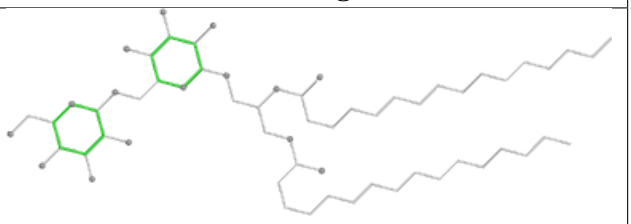
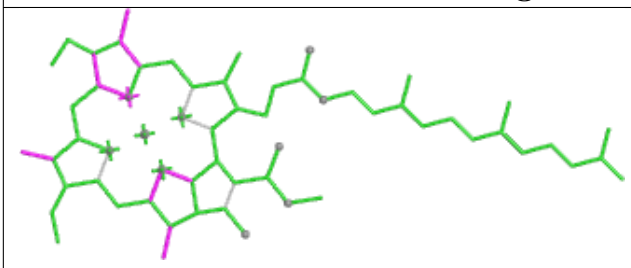


Rings

Ligand CLA Ba 313



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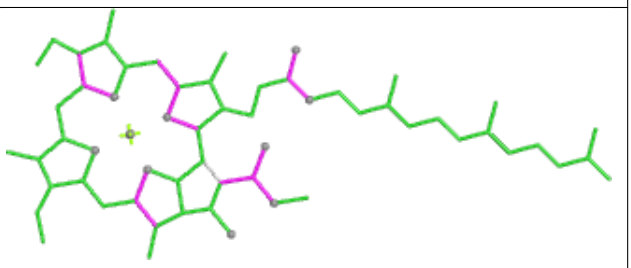
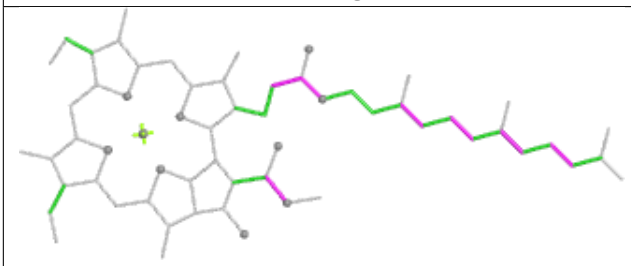


Bond angles



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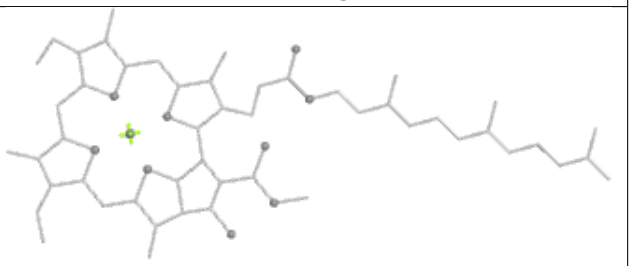
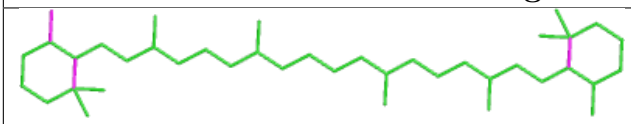


Rings

Ligand BCR F 101



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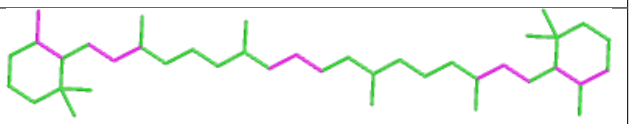

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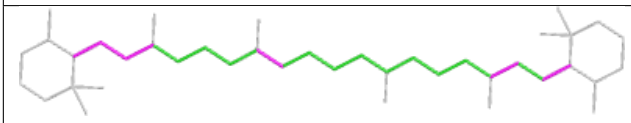

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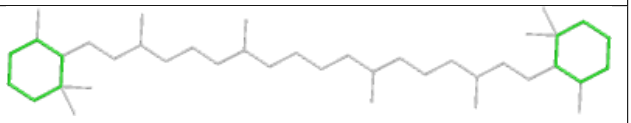
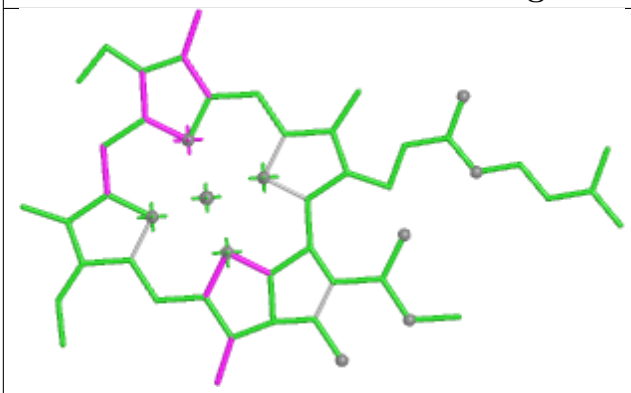


Rings

Ligand CLA n 604



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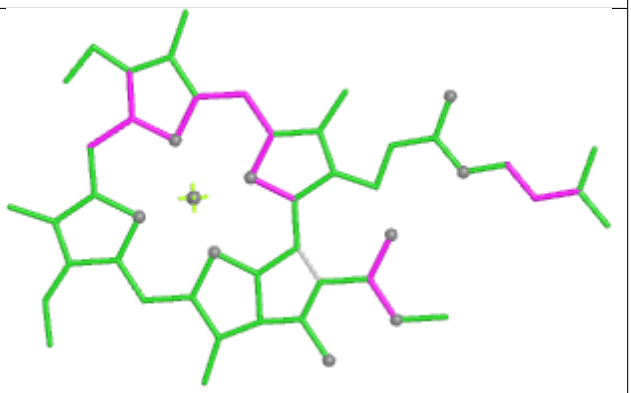
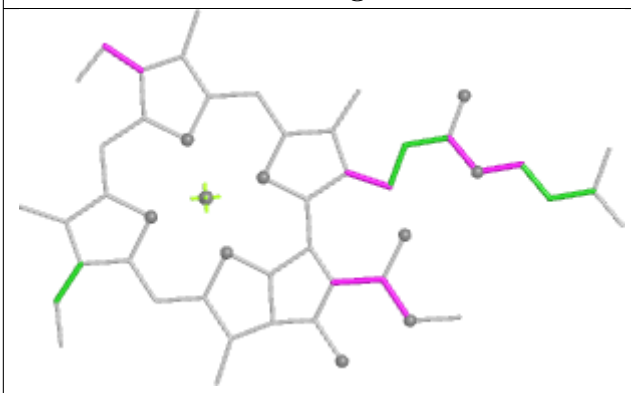


Bond angles



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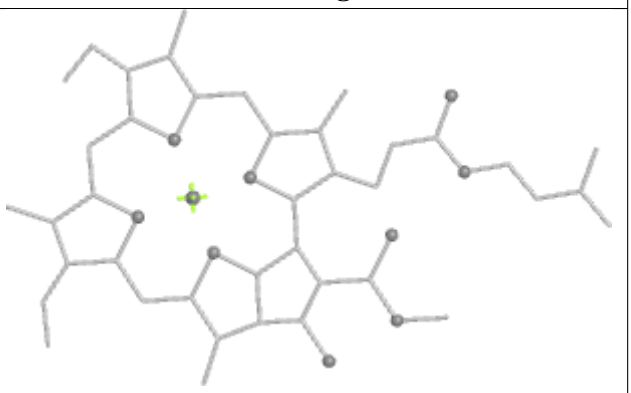
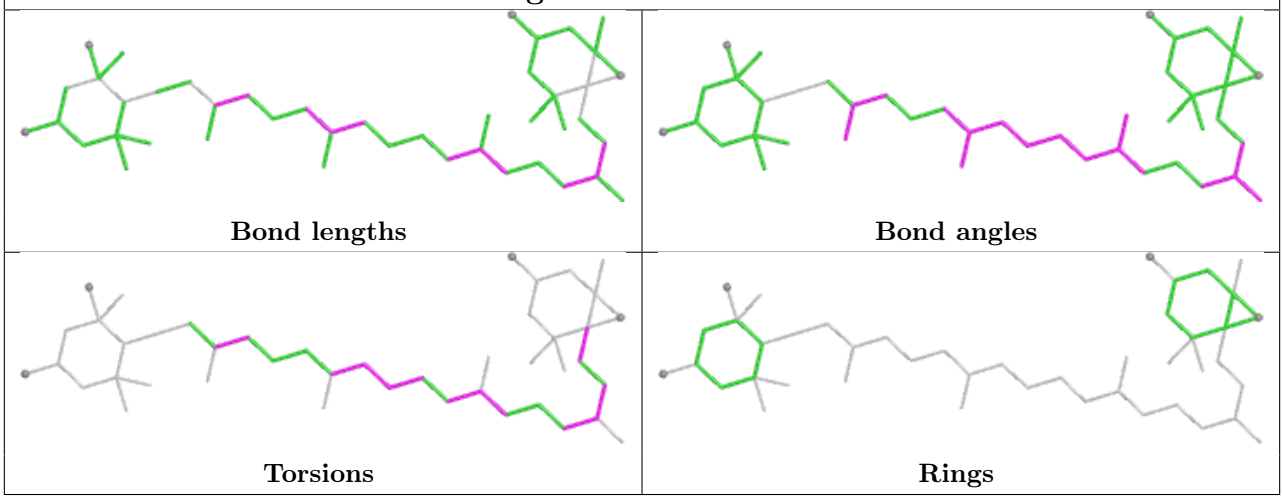
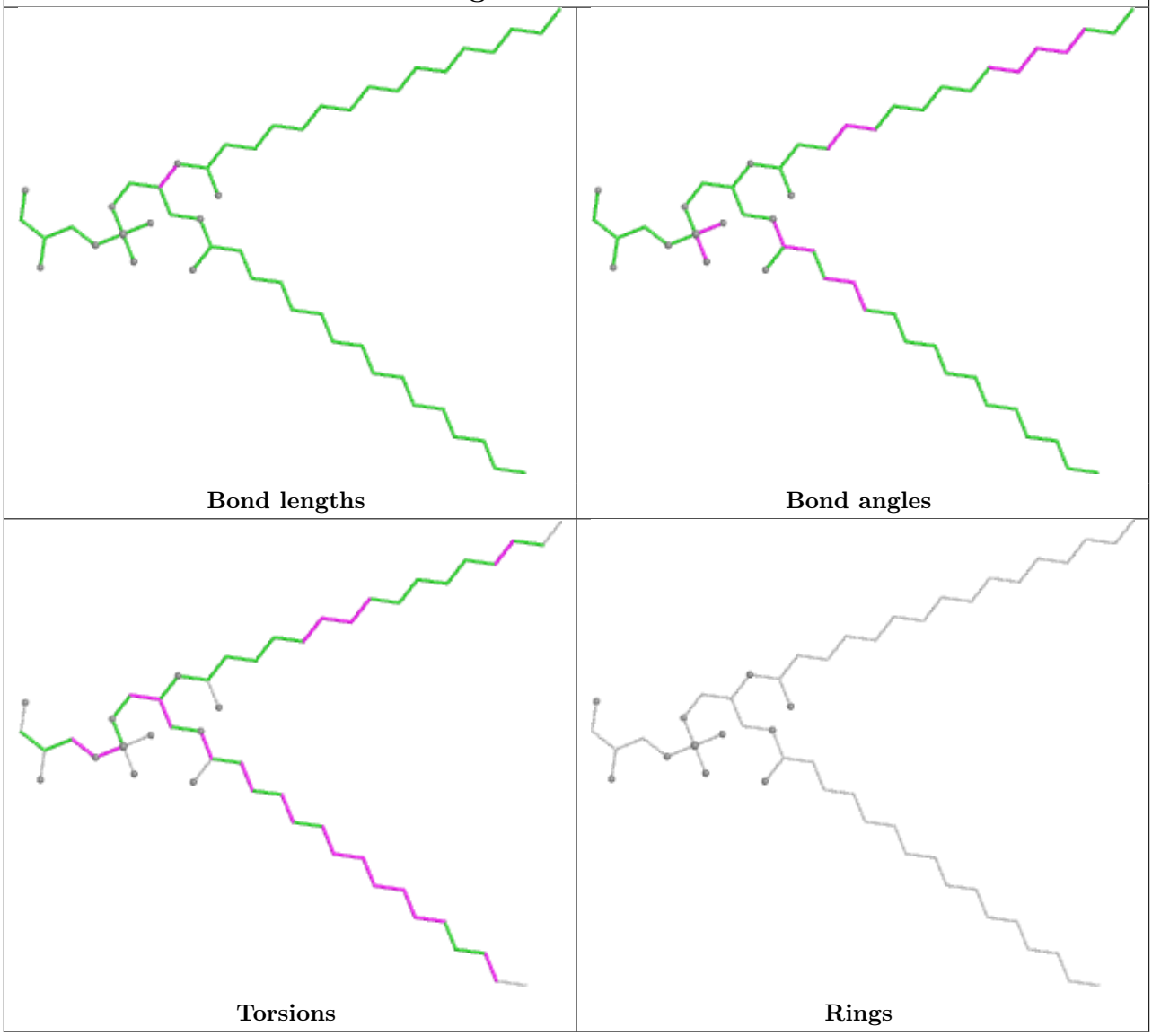


Rings

Ligand NEX n 617



Ligand LHG Y 319



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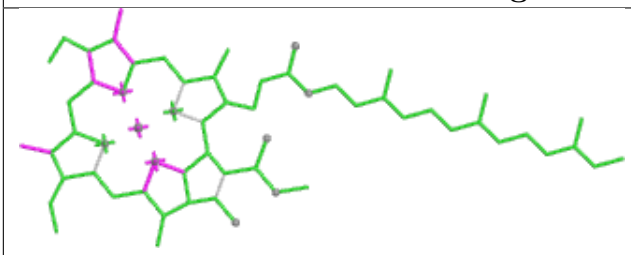

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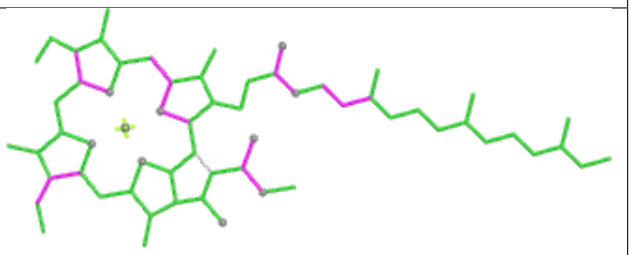
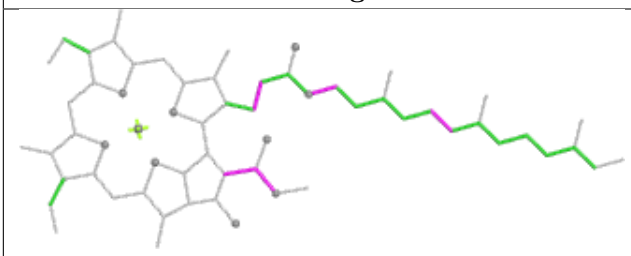


Bond angles



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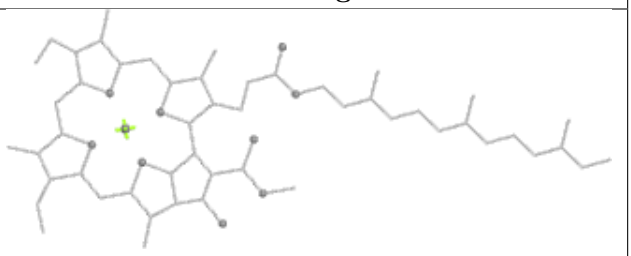
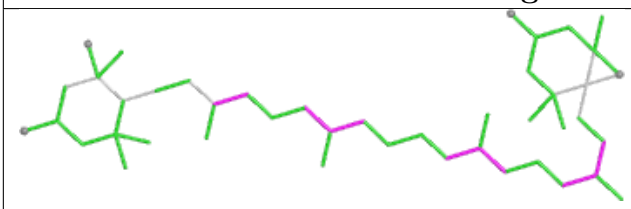


Rings

Ligand NEX N 617



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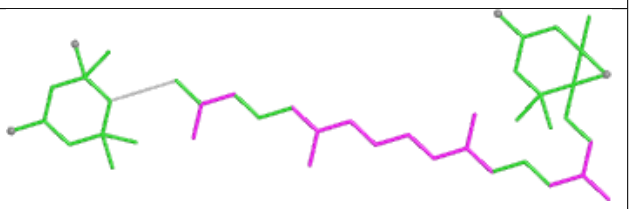

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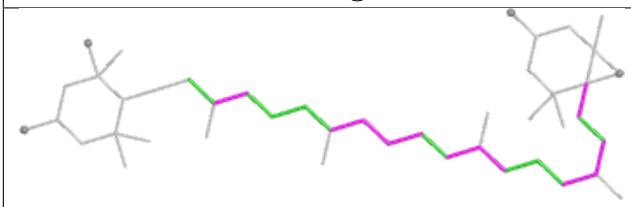

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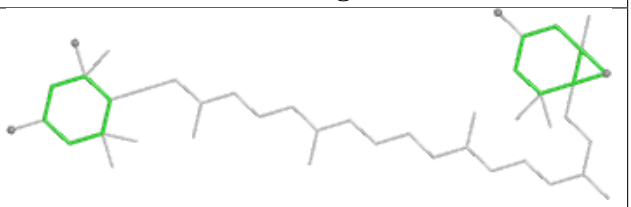
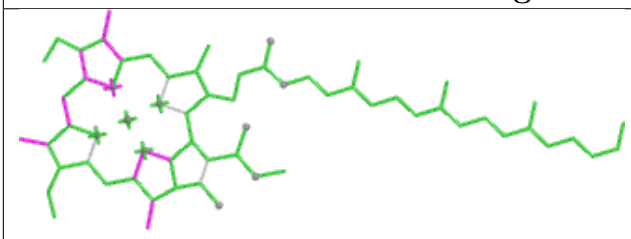


Rings

Ligand CLA Au 610



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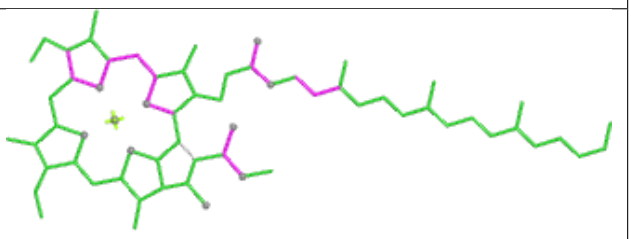
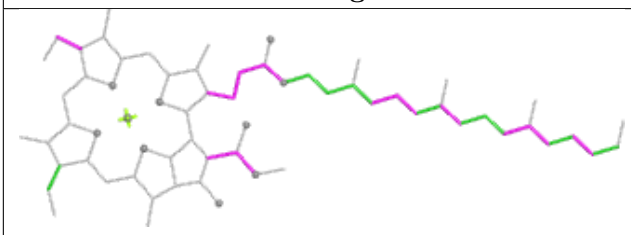


Bond angles



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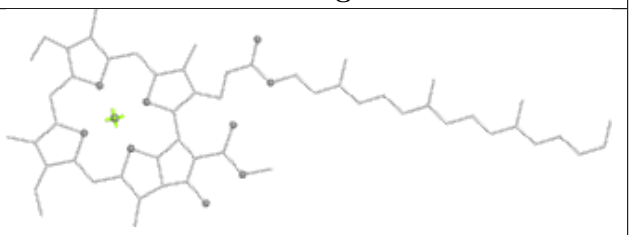
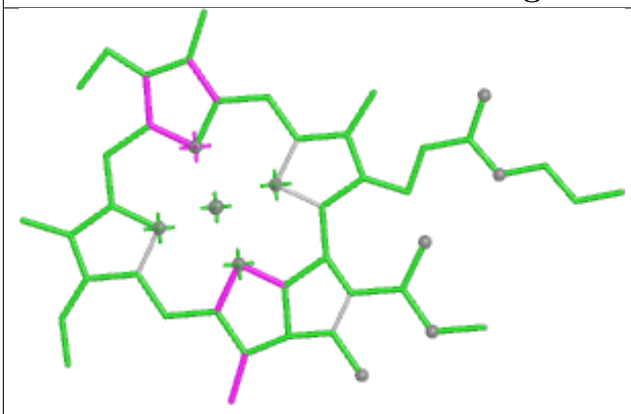
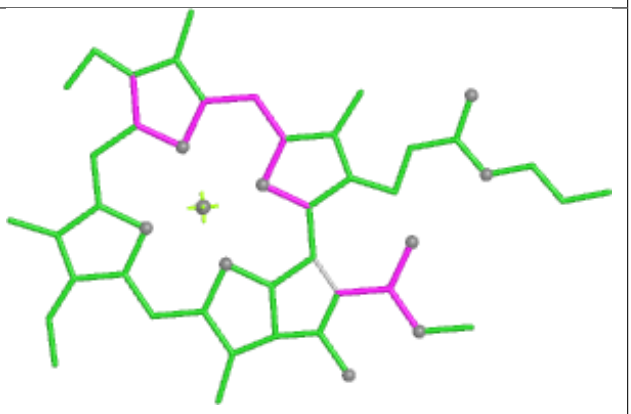
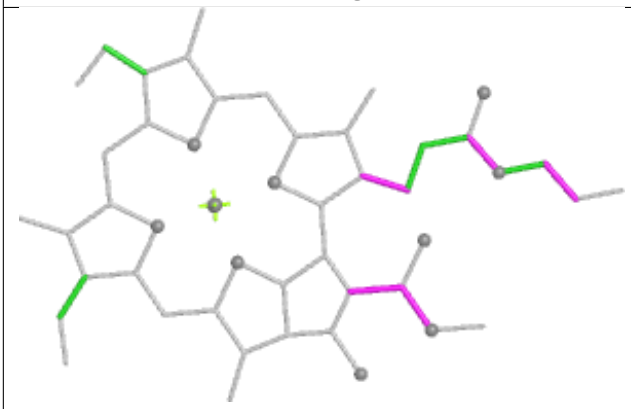
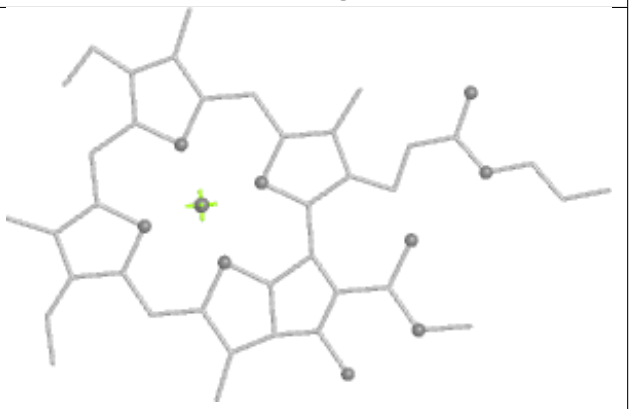


Rings

Ligand CLA N 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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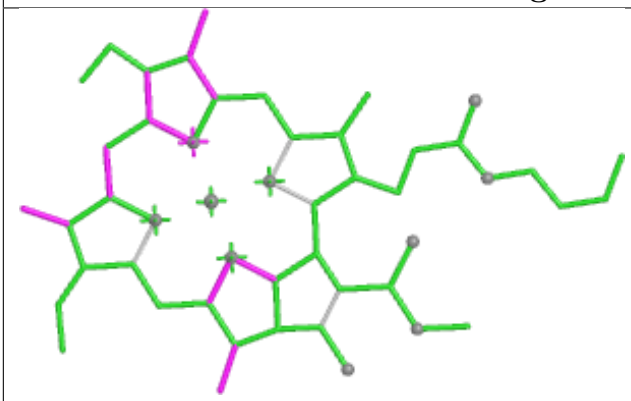
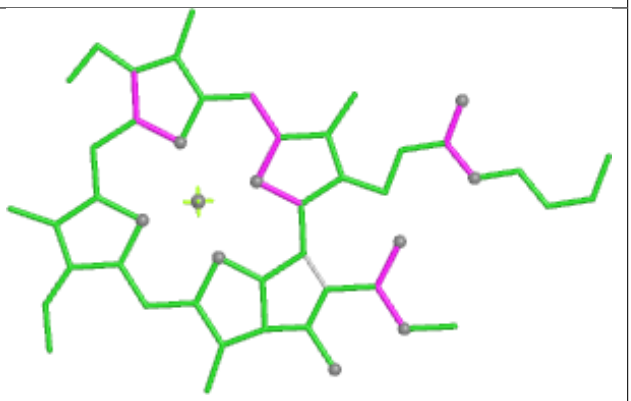
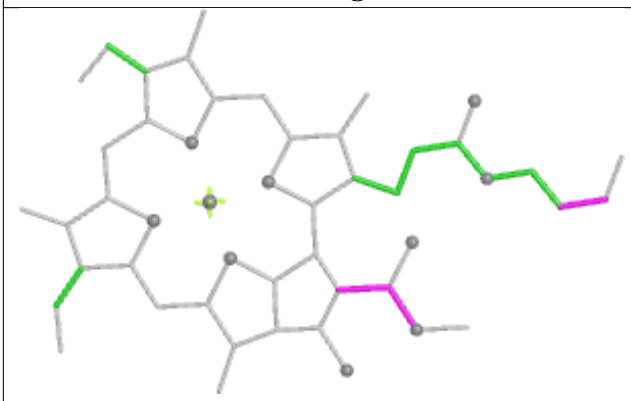
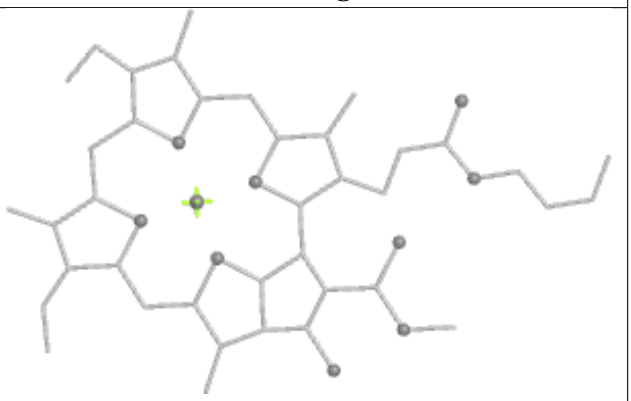
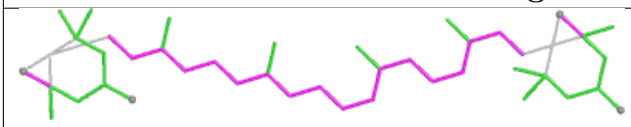
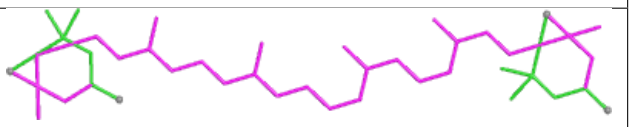
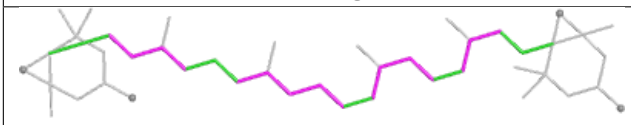
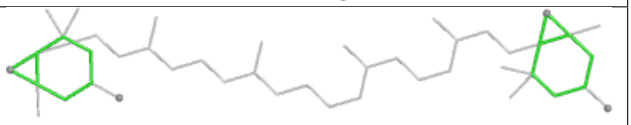
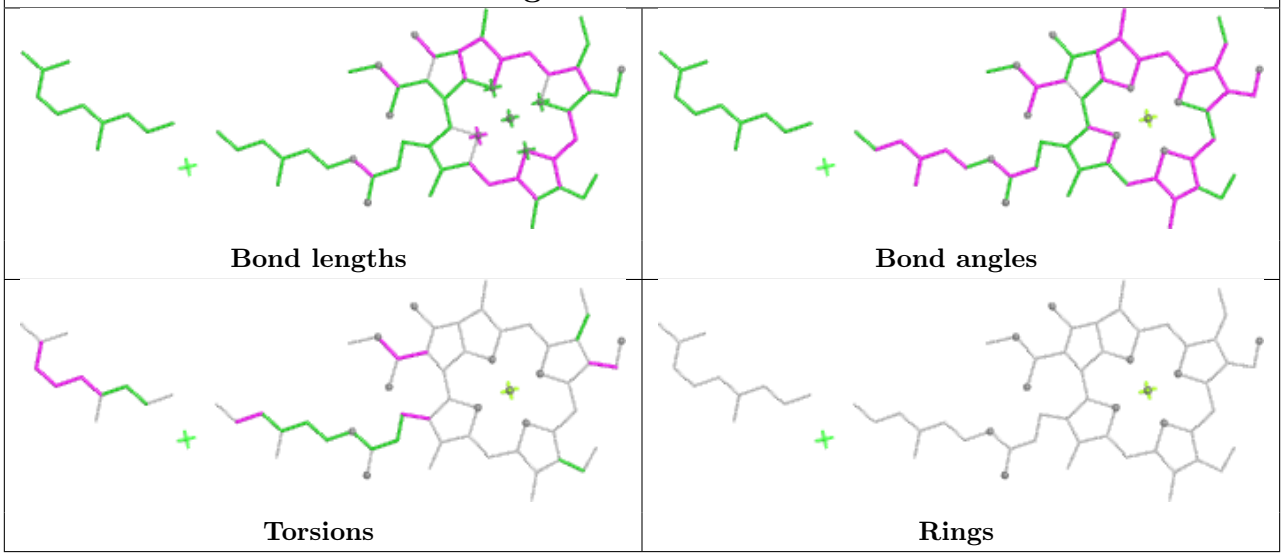
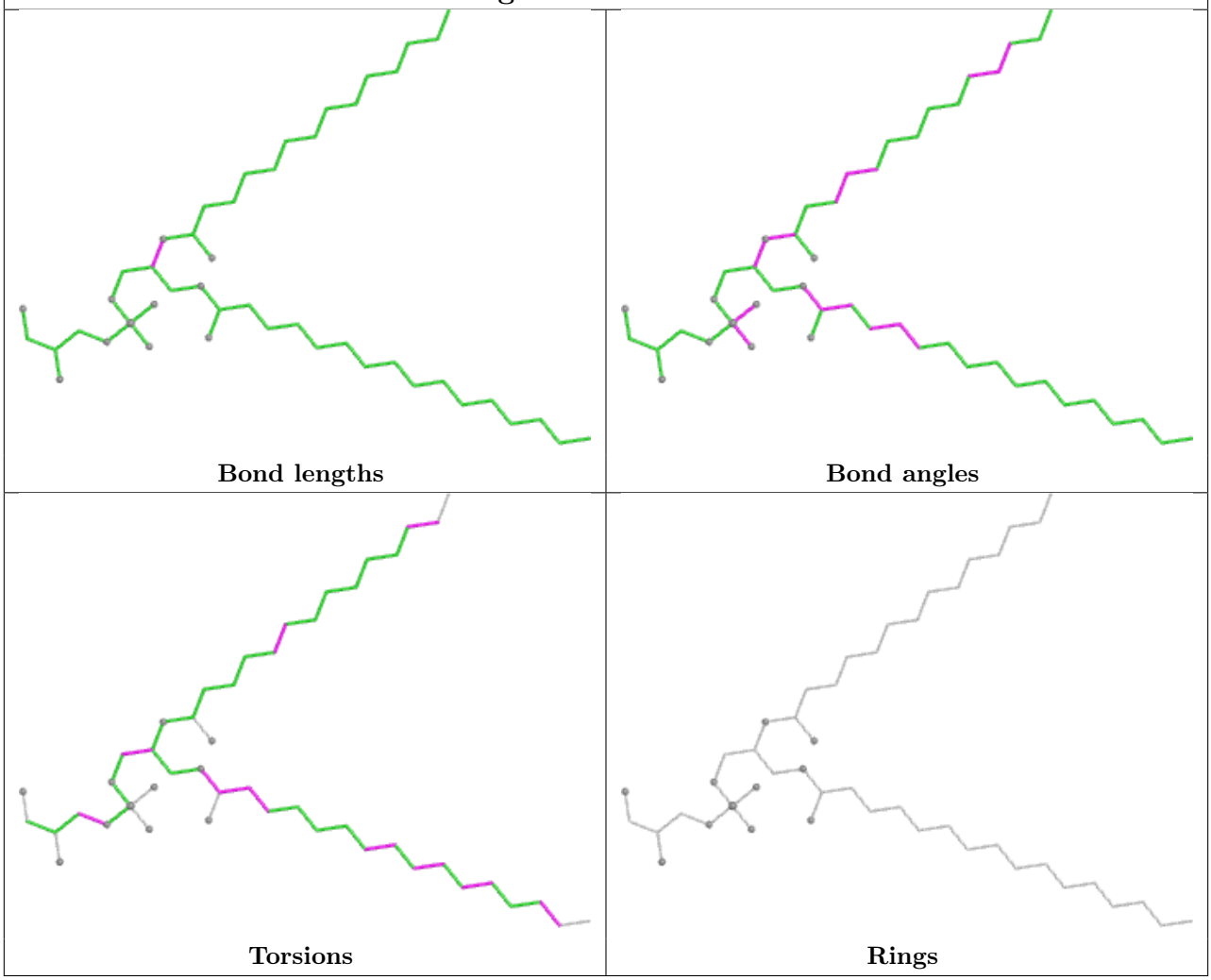
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 5 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 608



Ligand LHG 0 617



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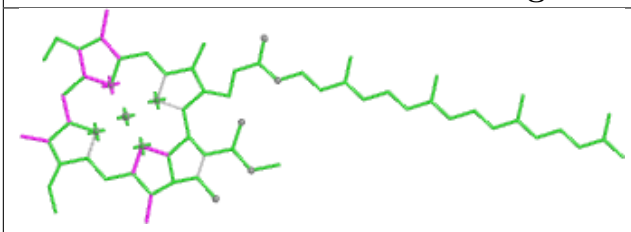
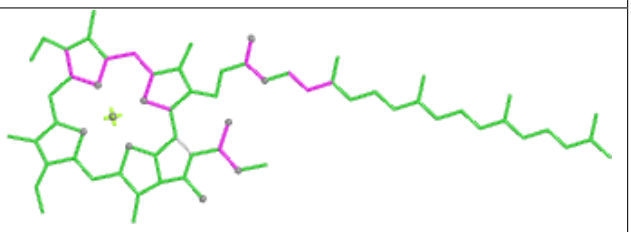
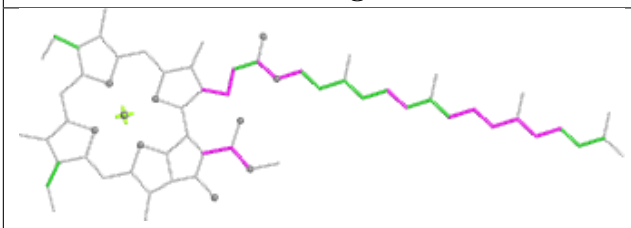
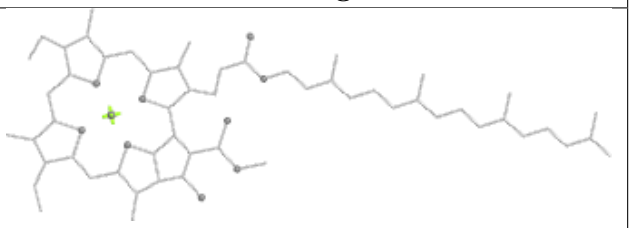
 Bond lengths	 Bond angles
 Torsions	 Rings

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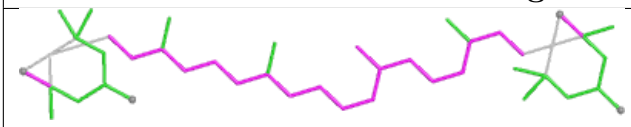
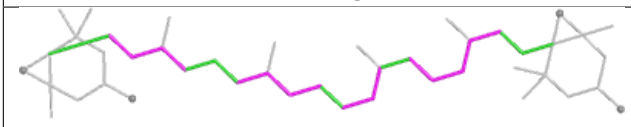
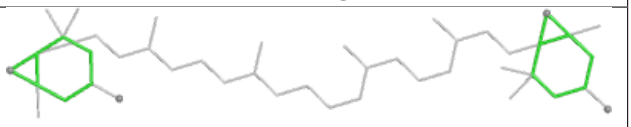
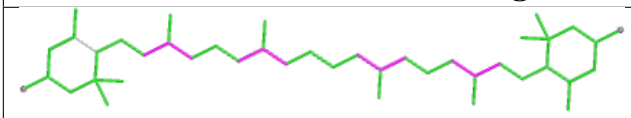
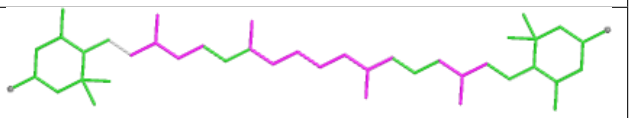
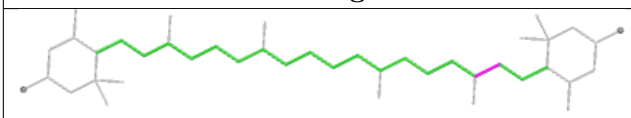
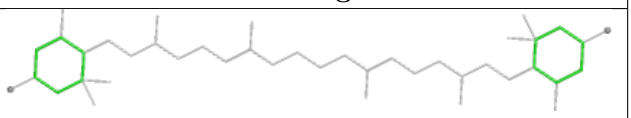
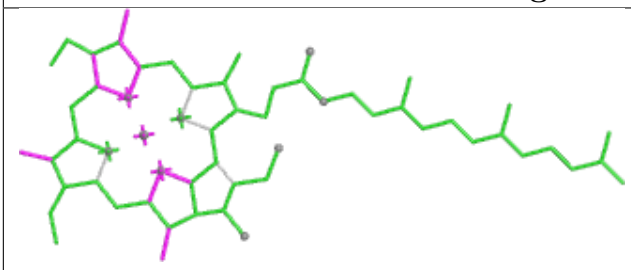
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand LUT BV 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 602



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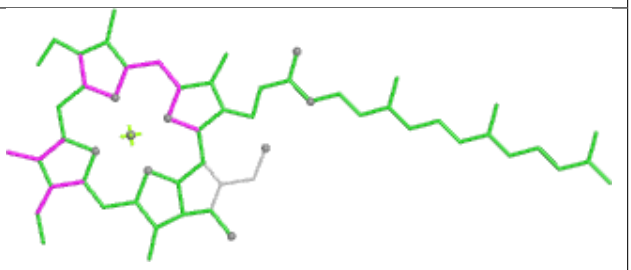
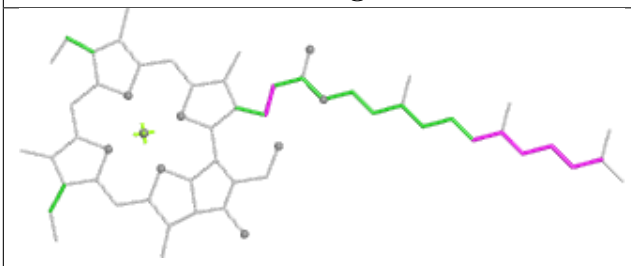


Bond angles



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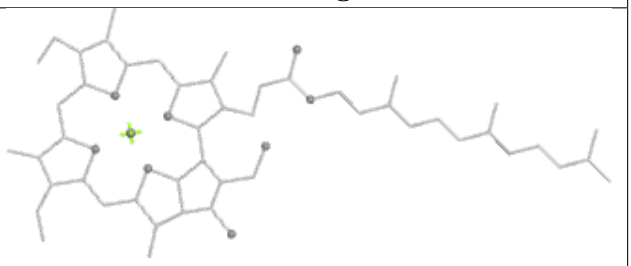
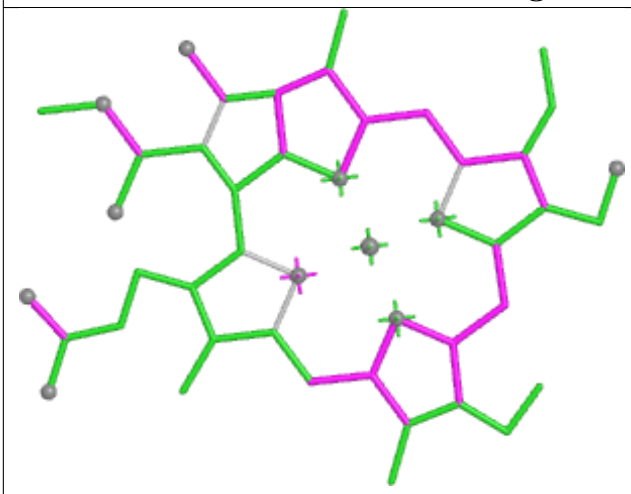


Rings

Ligand CHL 5 605



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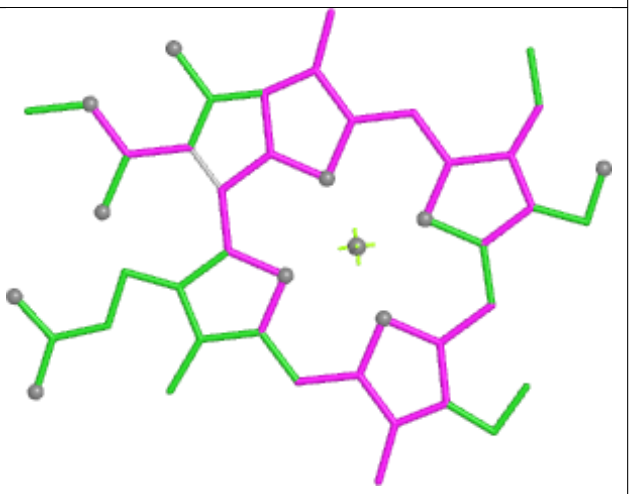
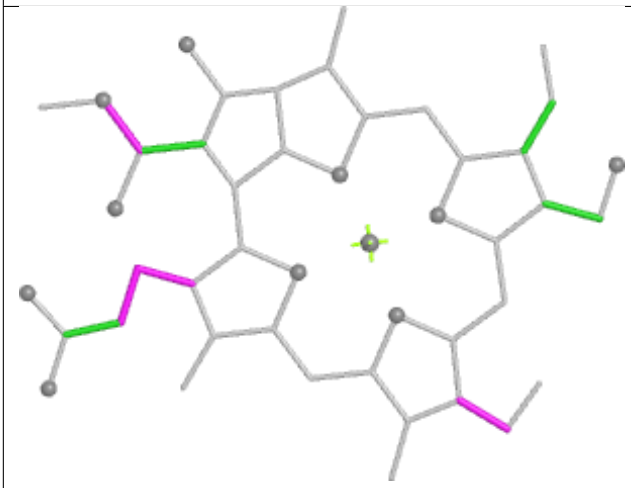


Bond angles



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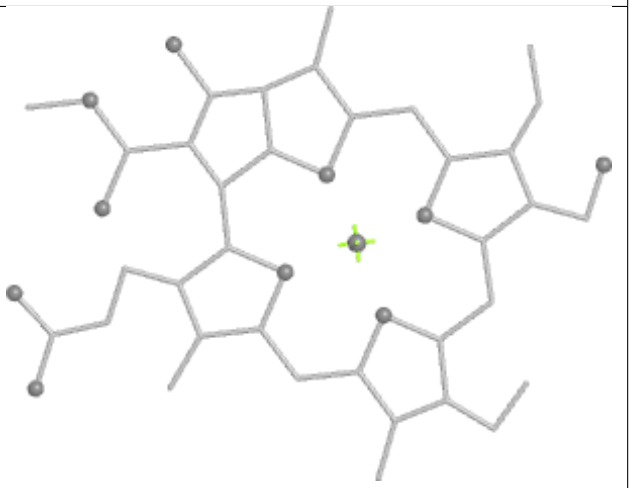
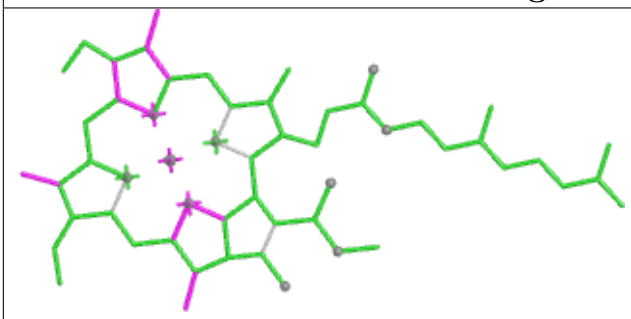


Rings

Ligand CLA 5 603



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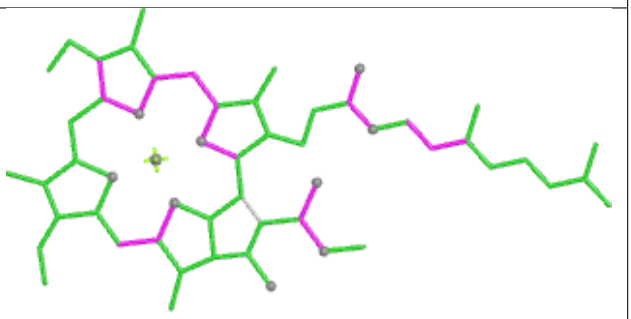

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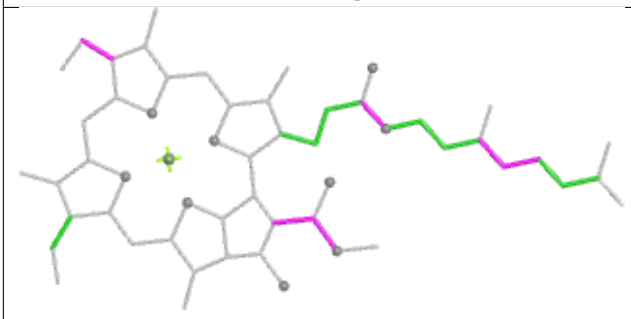

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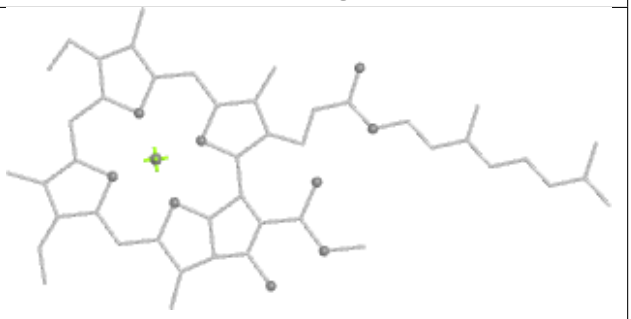
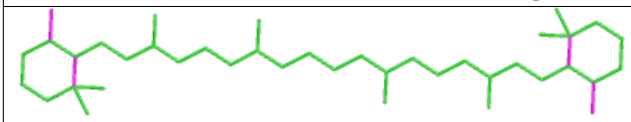


Rings

Ligand BCR z 101



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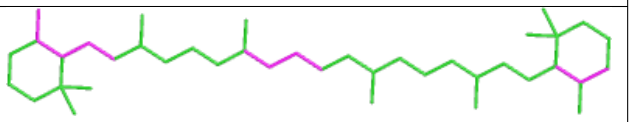
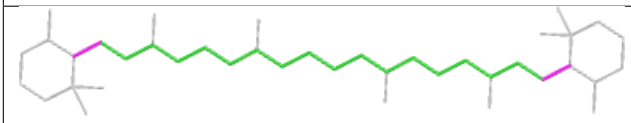


Bond angles



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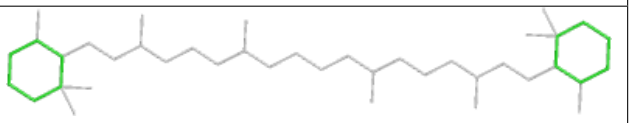
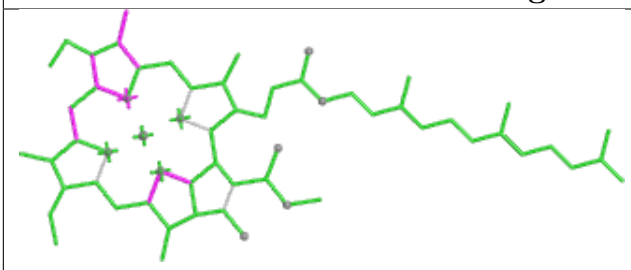


Rings

Ligand CLA g 611



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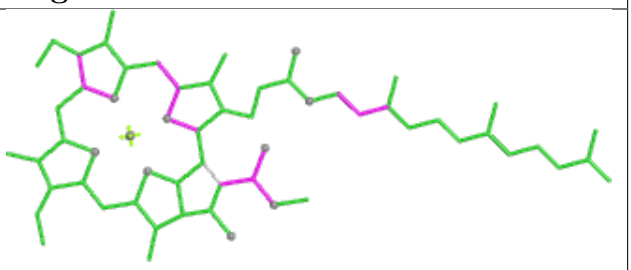
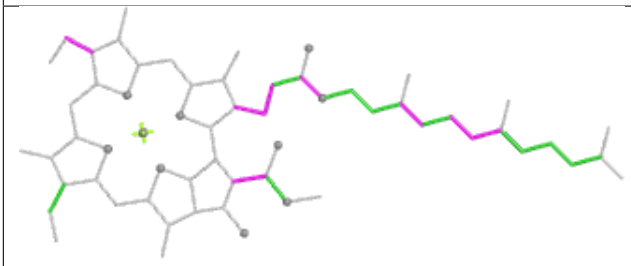


Bond angles



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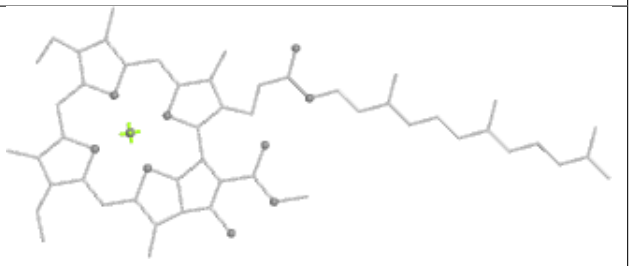
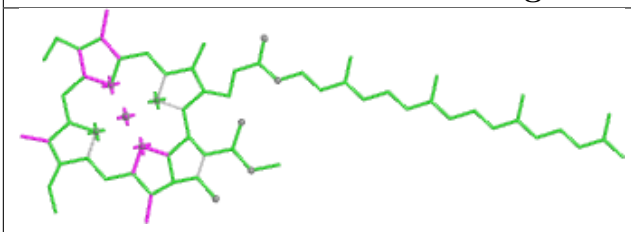
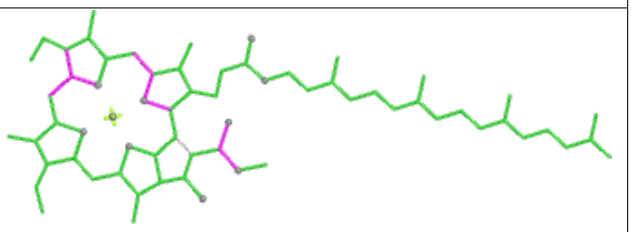
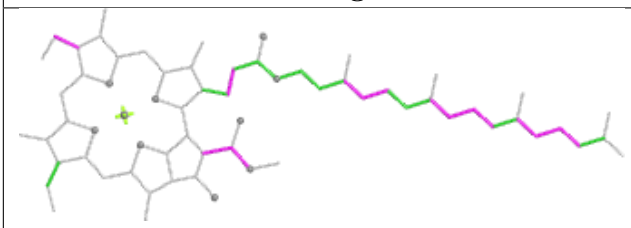
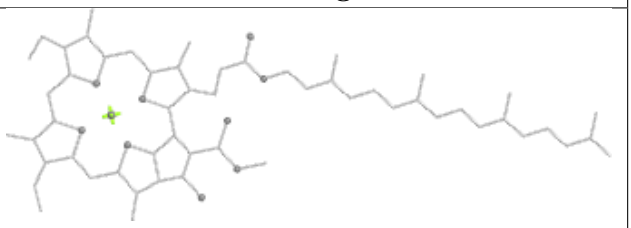
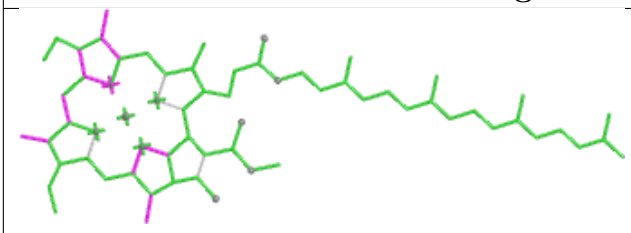
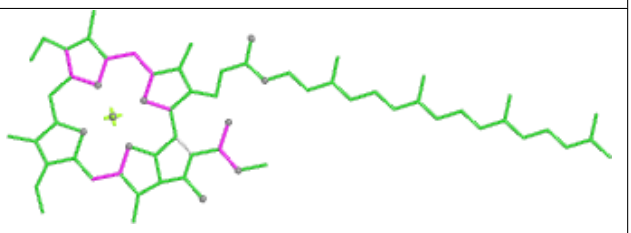
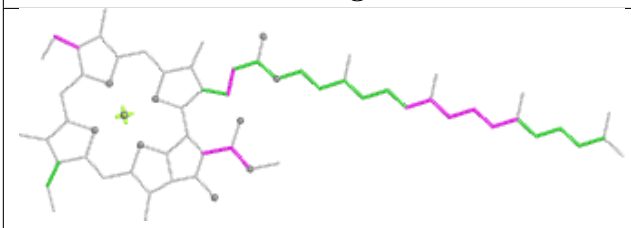
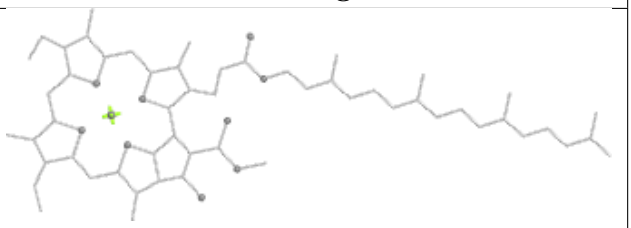
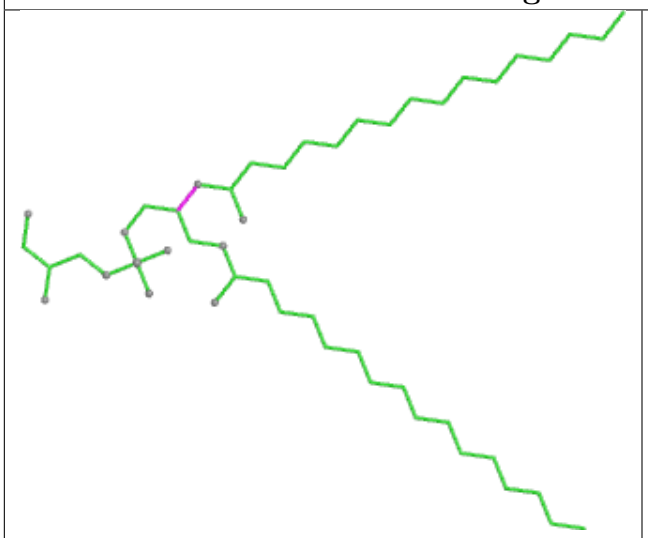


Rings

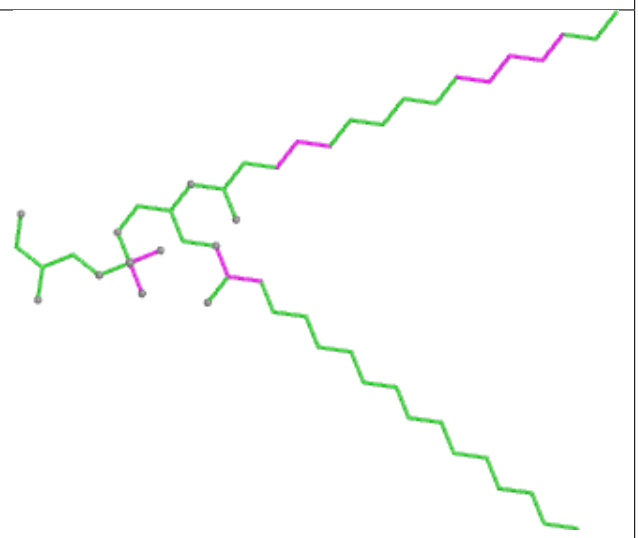
Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

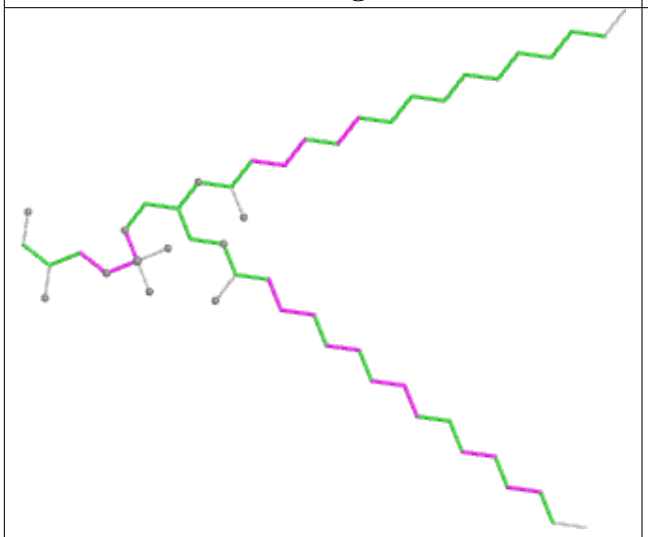
Ligand LHG D 404



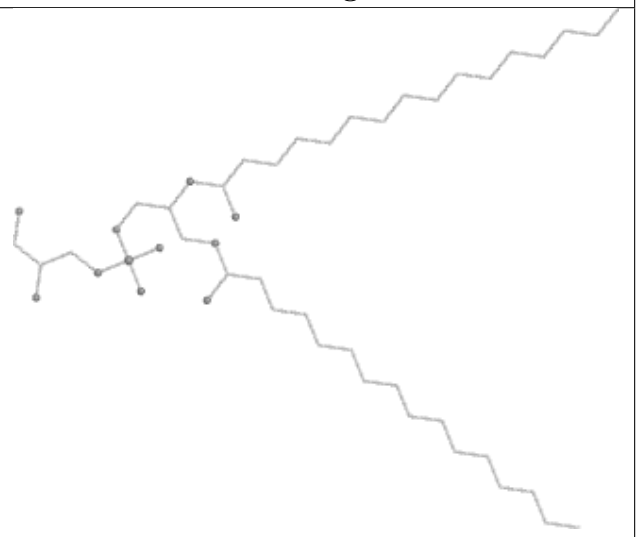
Bond lengths



Bond angles



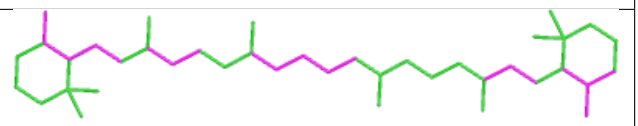
Torsions



Rings

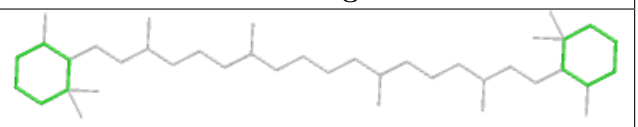
Ligand BCR z 102

Bond lengths

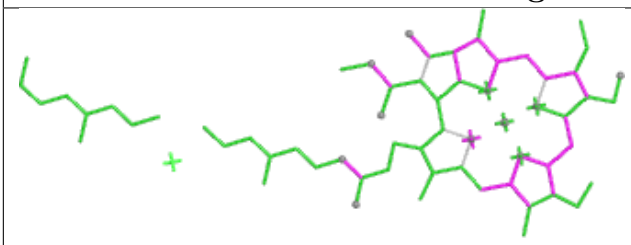
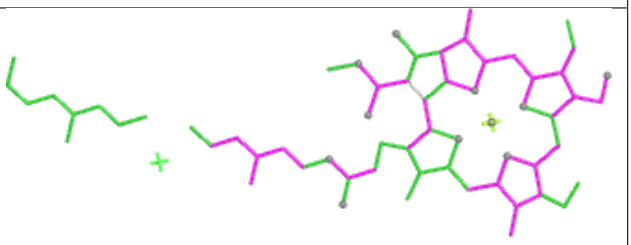
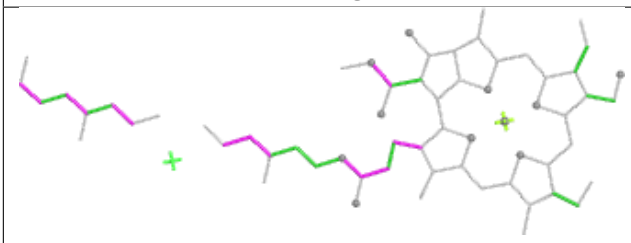
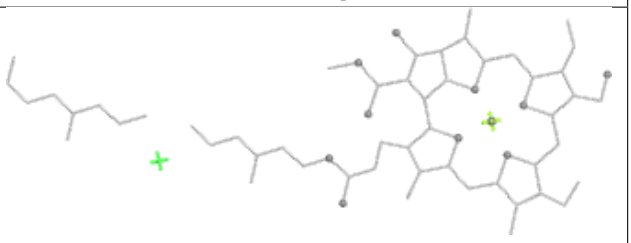


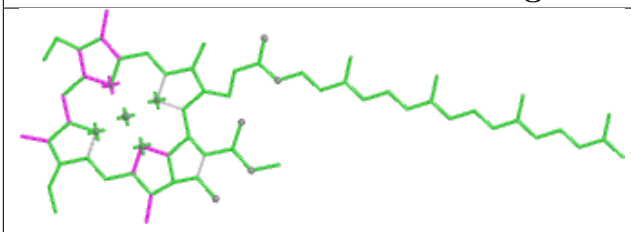
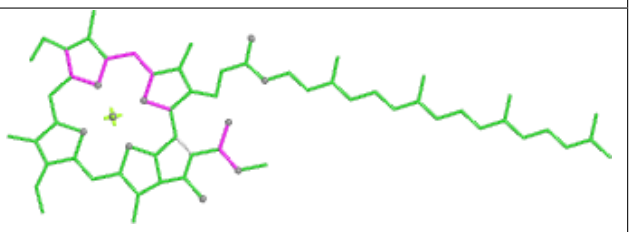
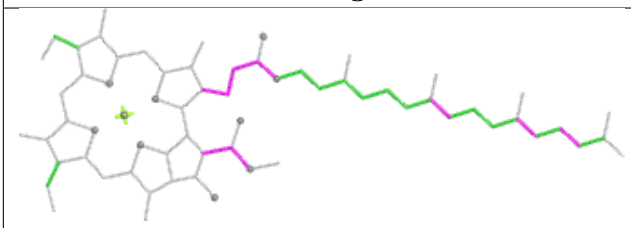
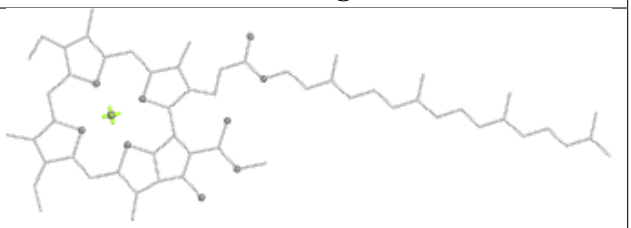
Bond angles

Torsions

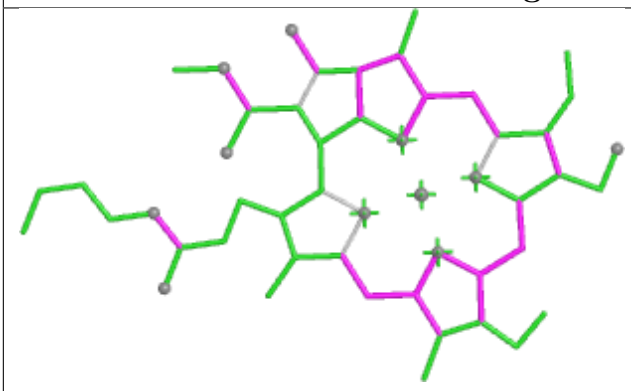


Rings

Ligand CHL 0 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Y 307



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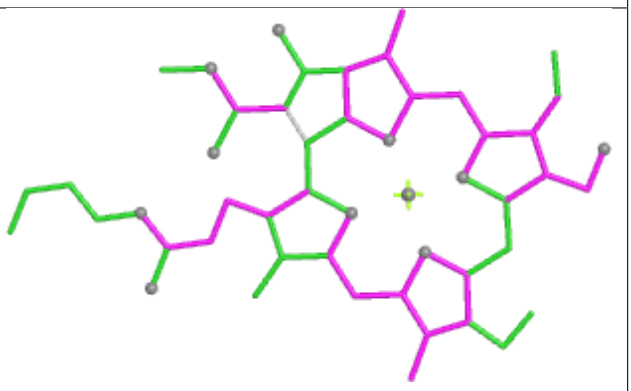

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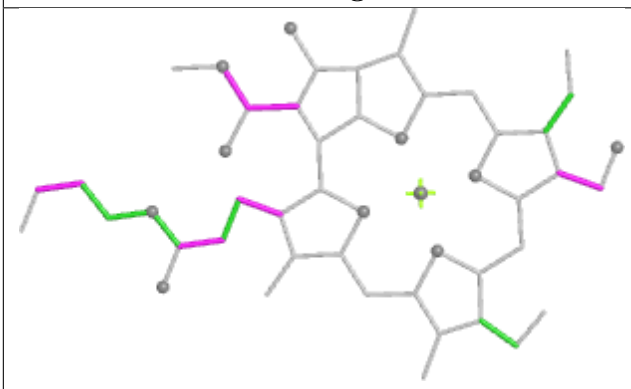

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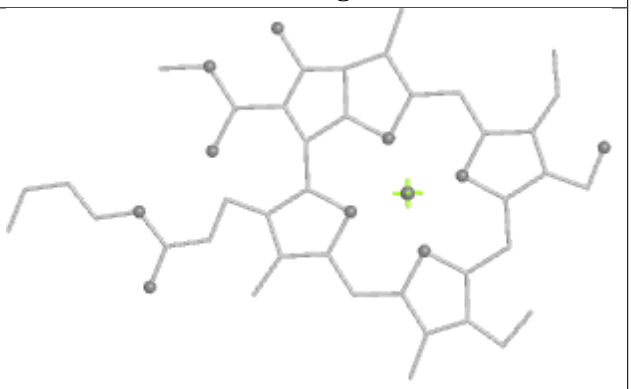
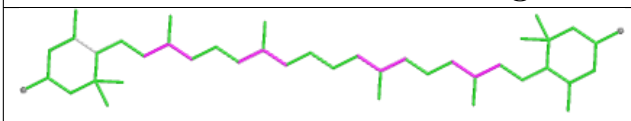


Rings

Ligand LUT BQ 616



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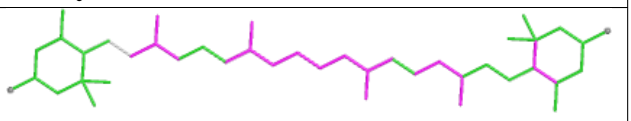

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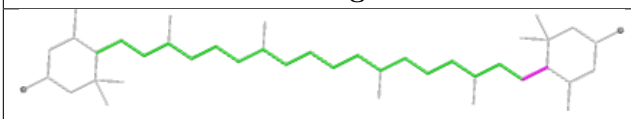

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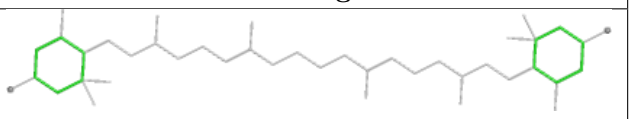
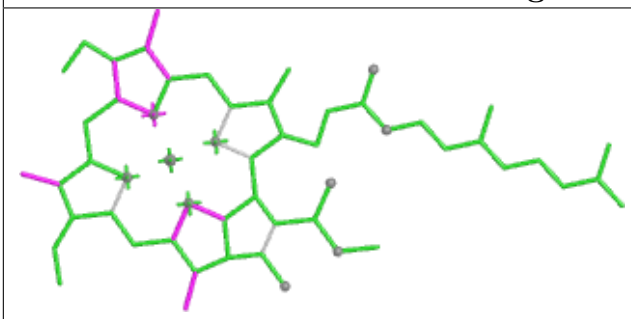


Rings

Ligand CLA S 612



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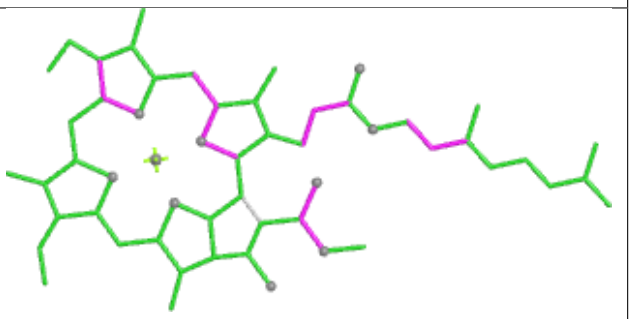

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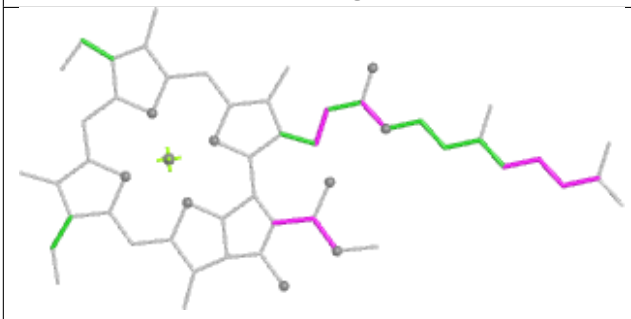

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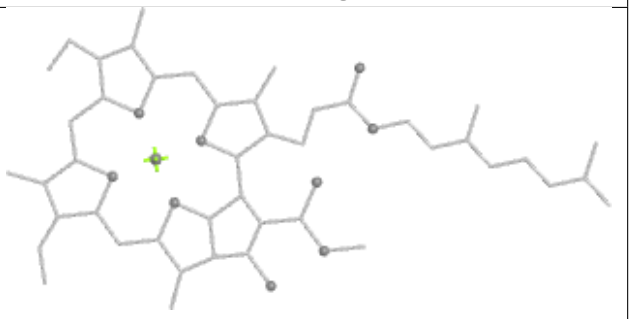
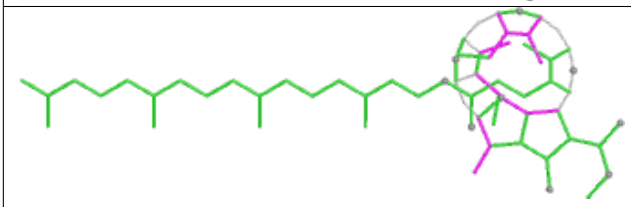


Rings

Ligand PHO A 408



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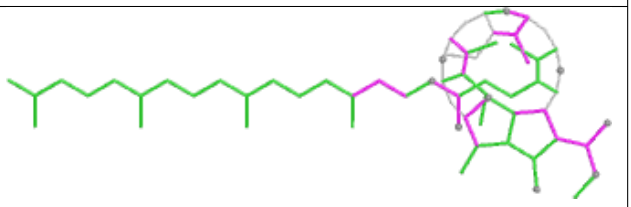

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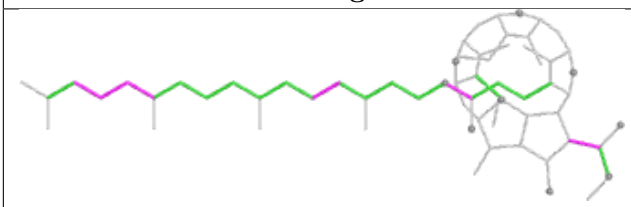

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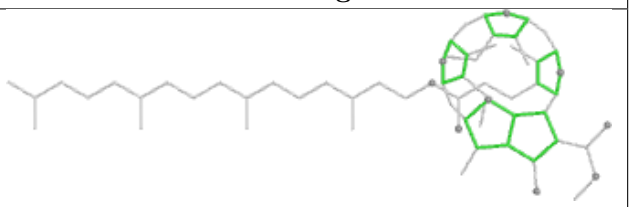
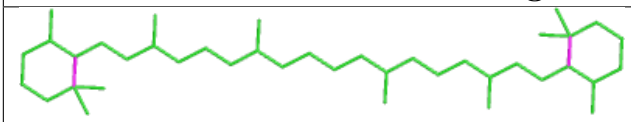


Rings

Ligand BCR v 622



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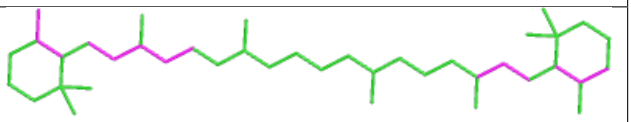

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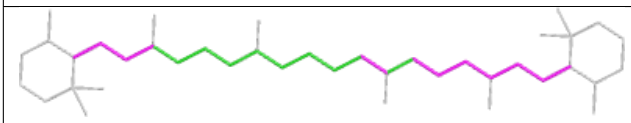

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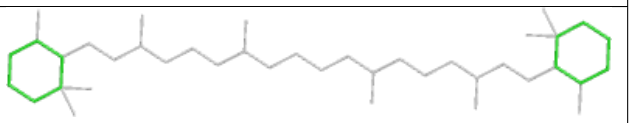
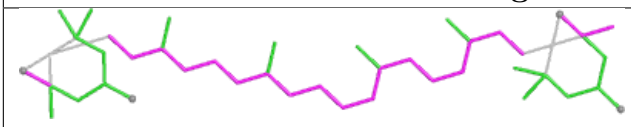
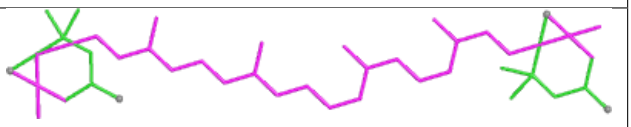
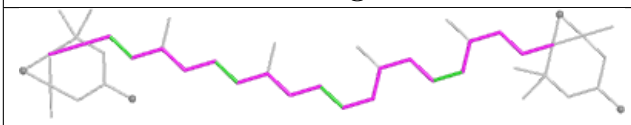
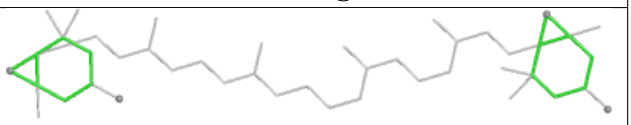
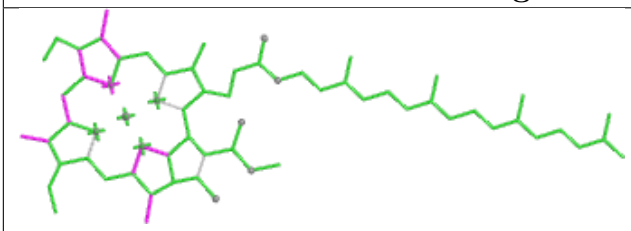
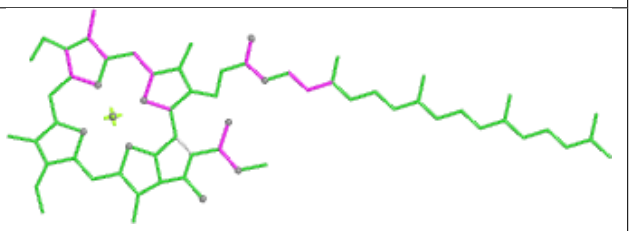
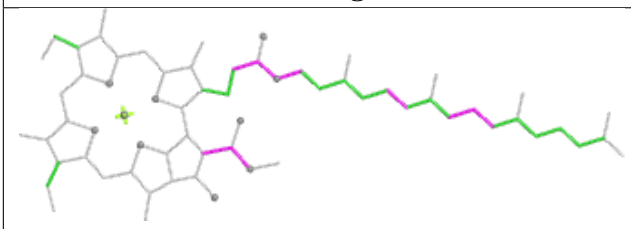
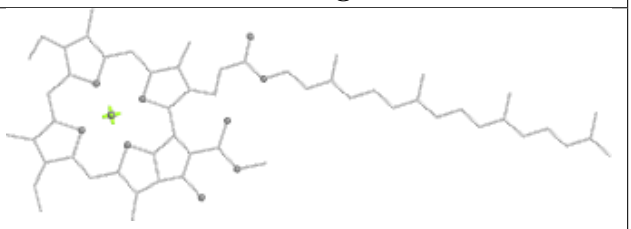


Rings

Ligand XAT BB 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BE 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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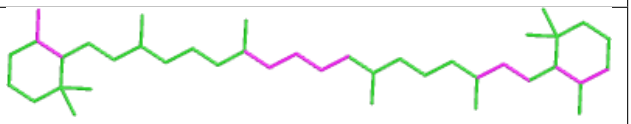
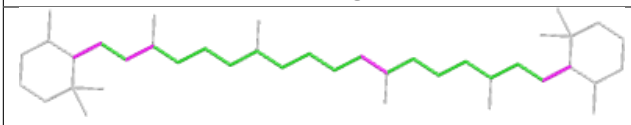
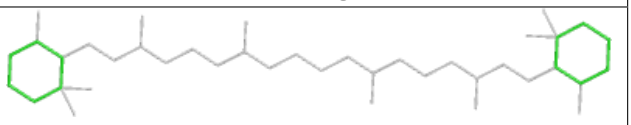
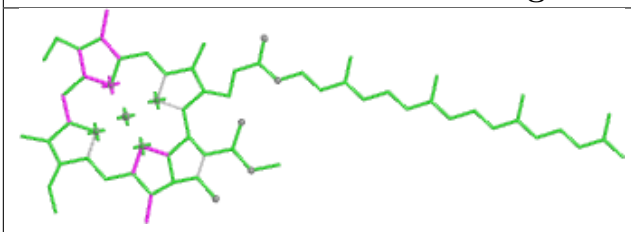
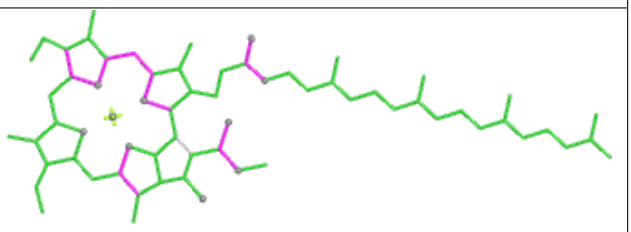
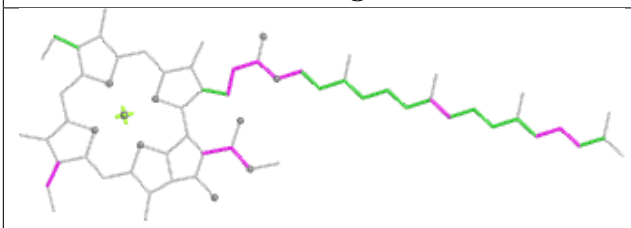
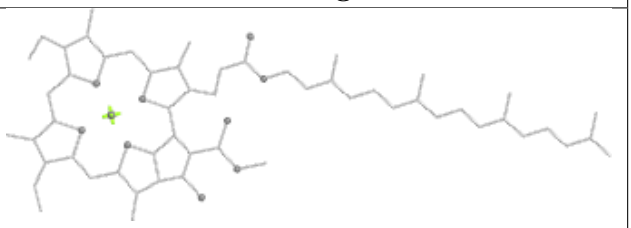
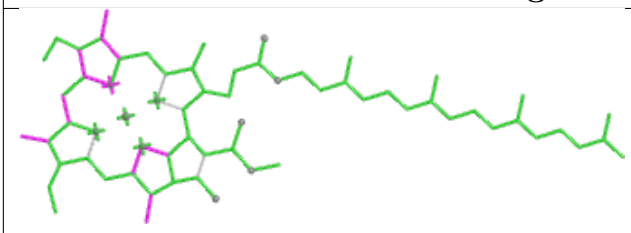
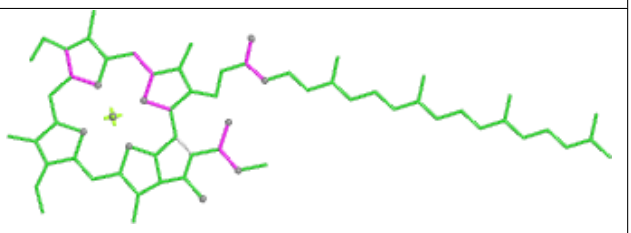
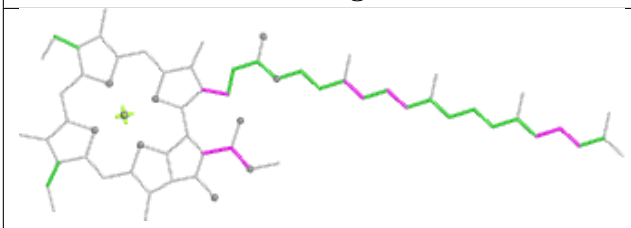
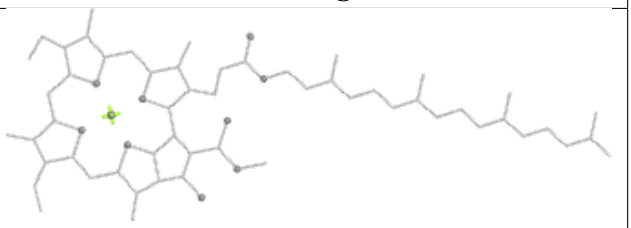
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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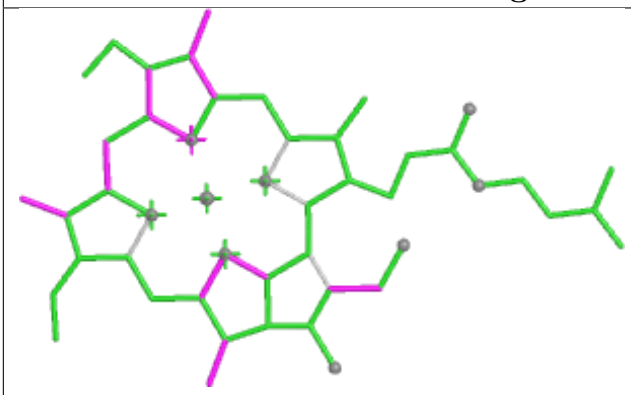	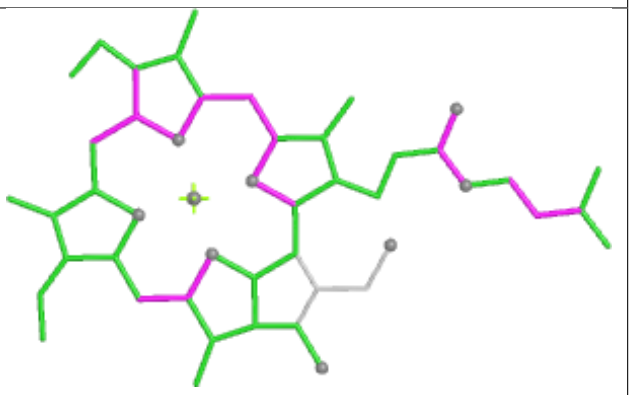
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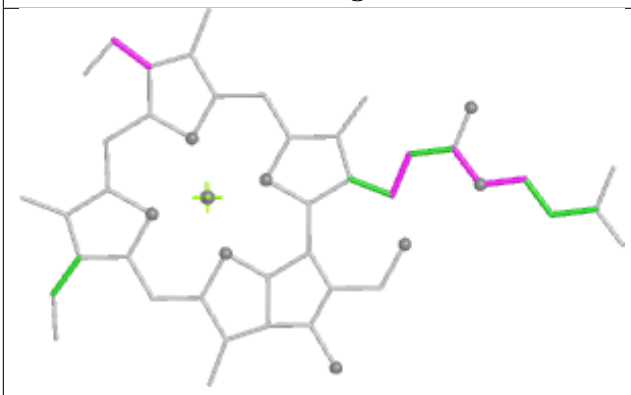
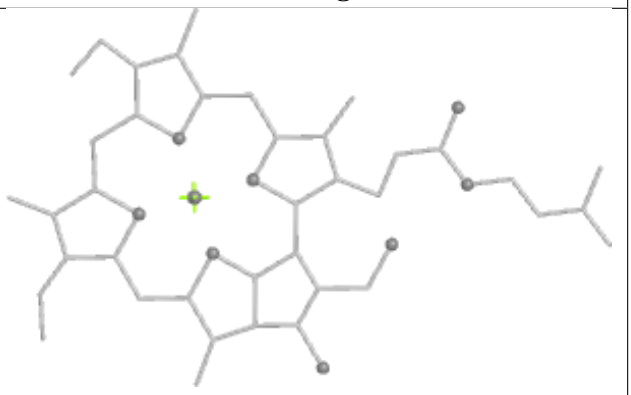
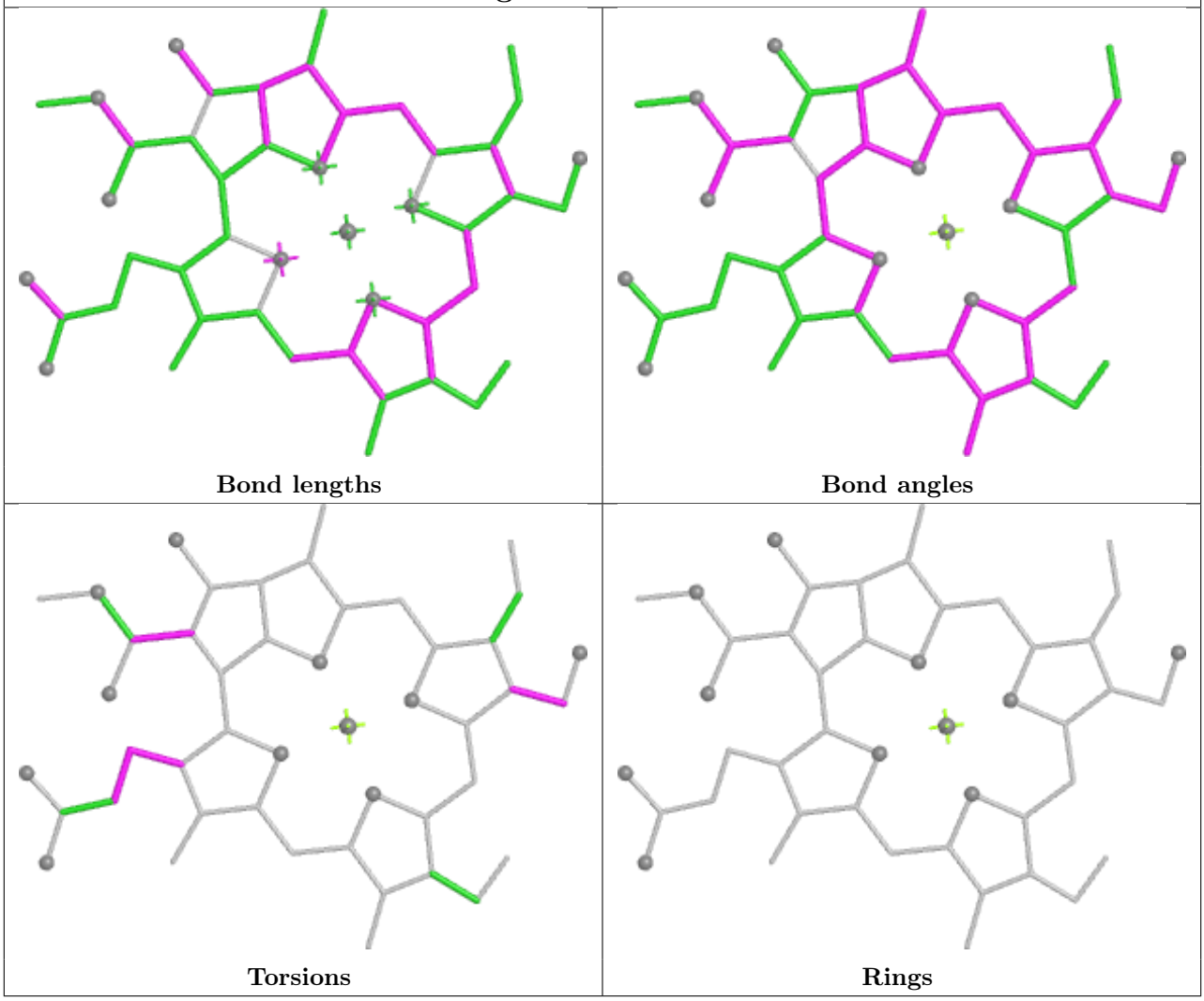
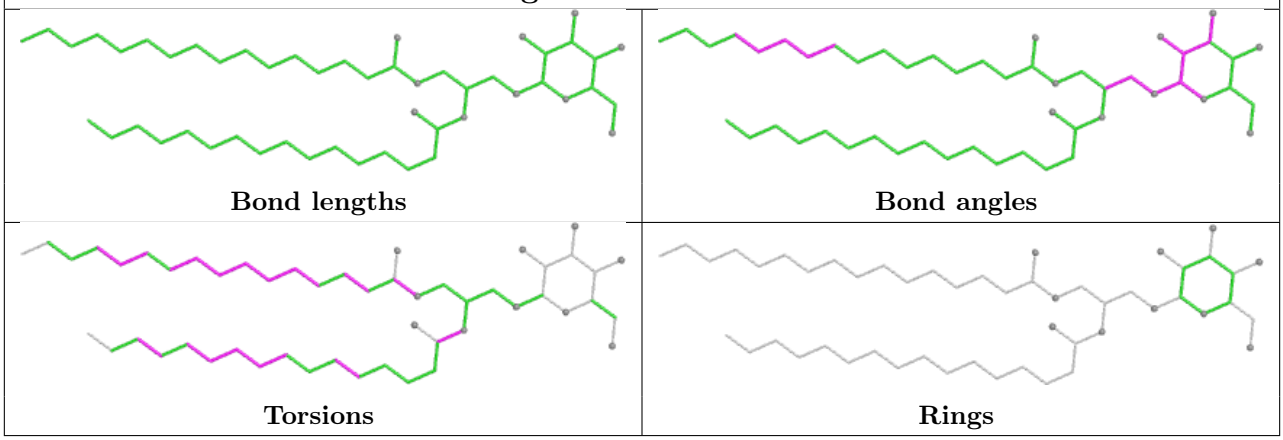
	
Torsions	**Rings**

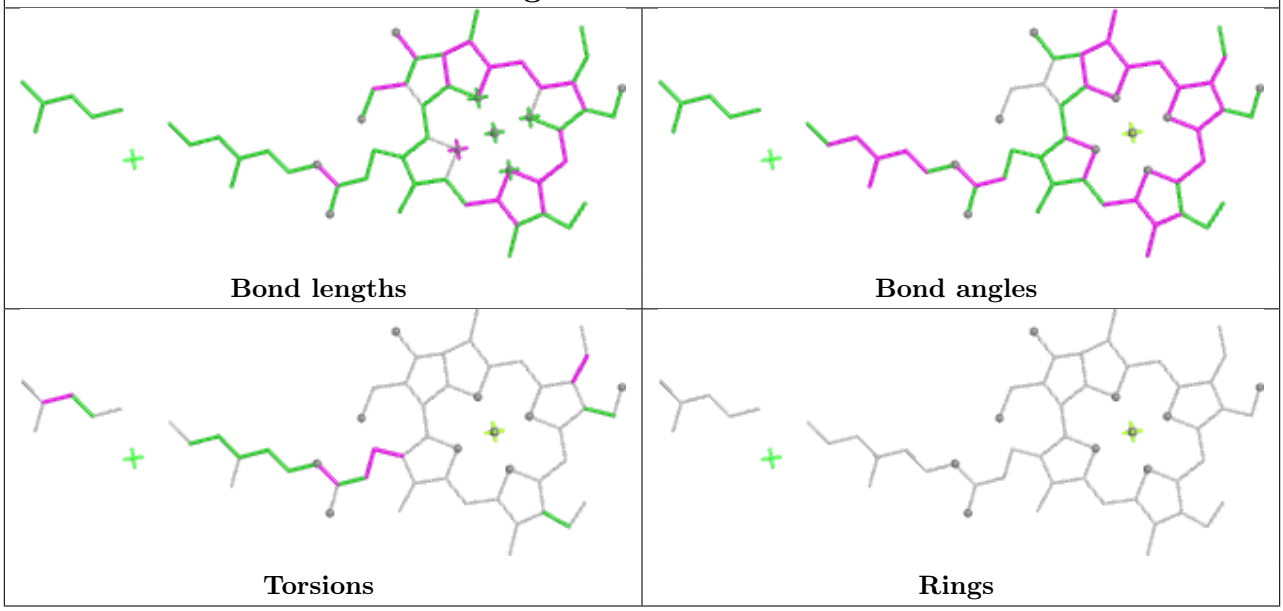
Ligand CHL 0 608



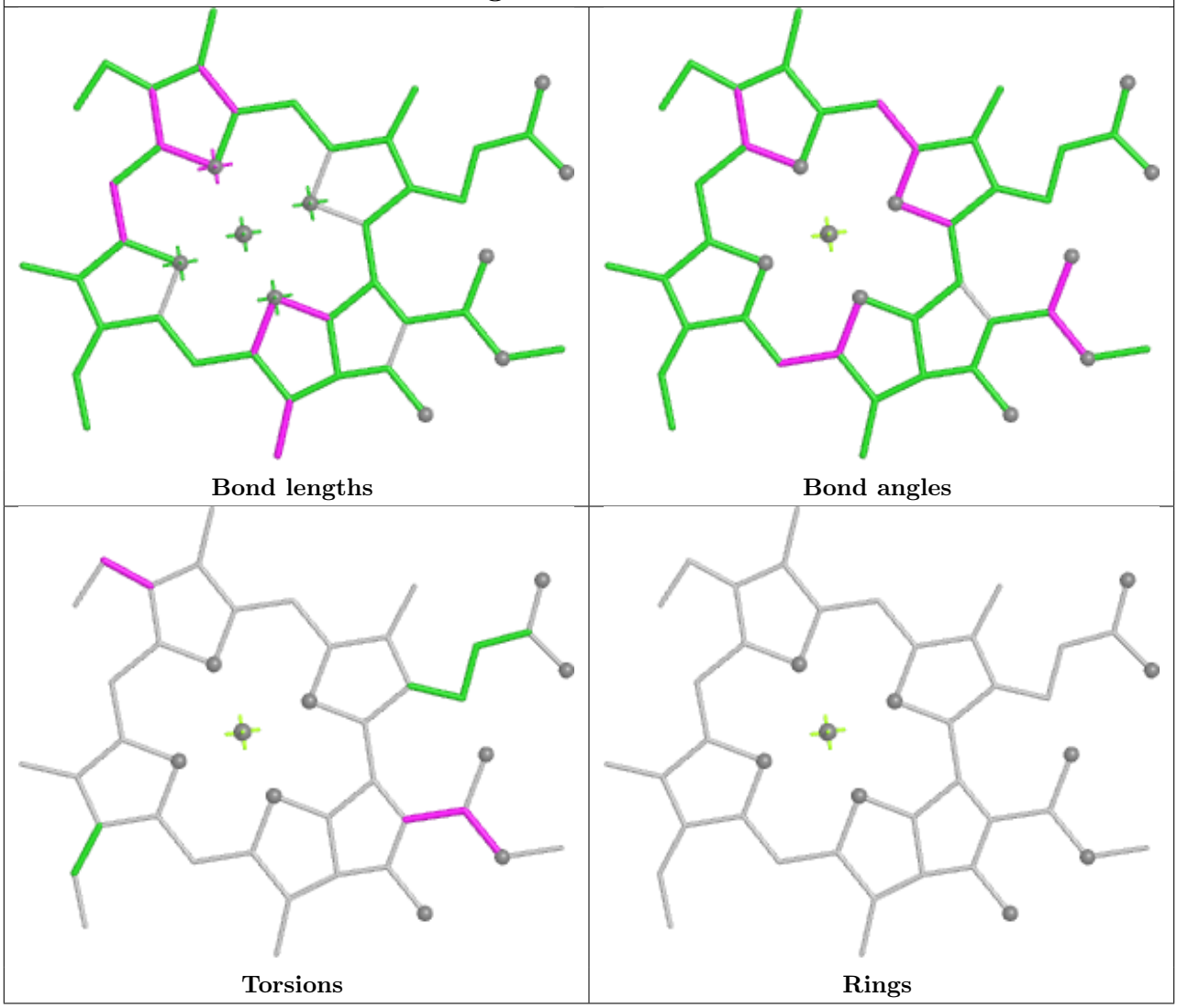
Ligand LMG B 620

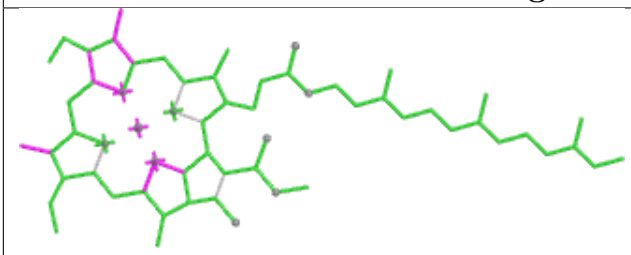
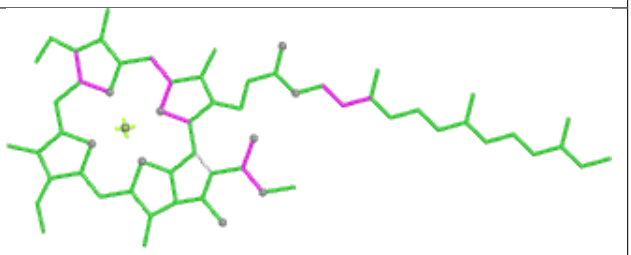
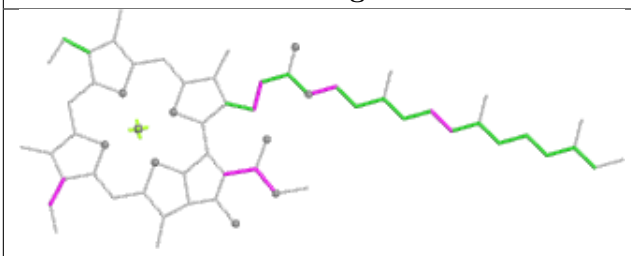
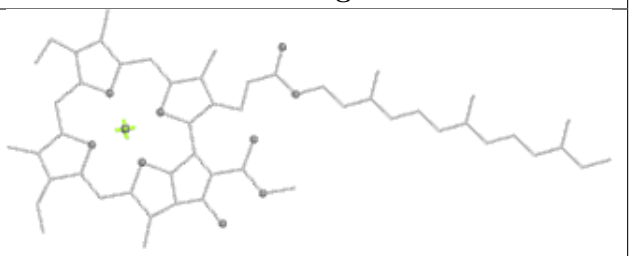


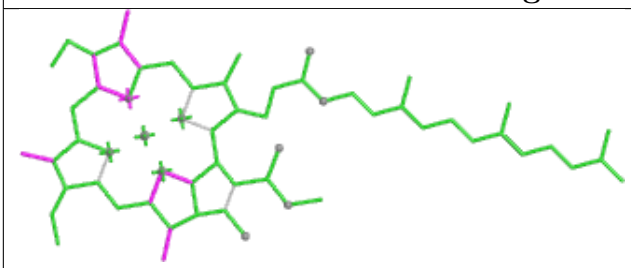
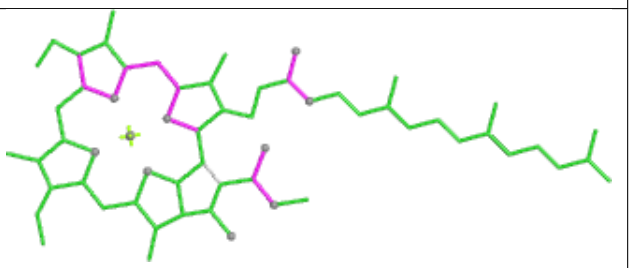
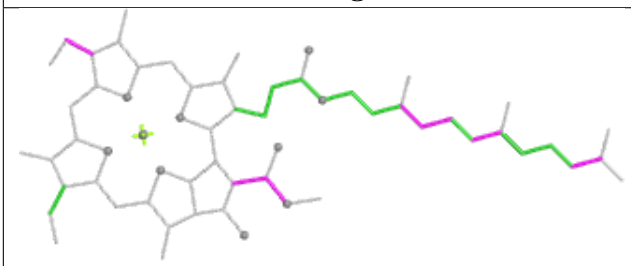
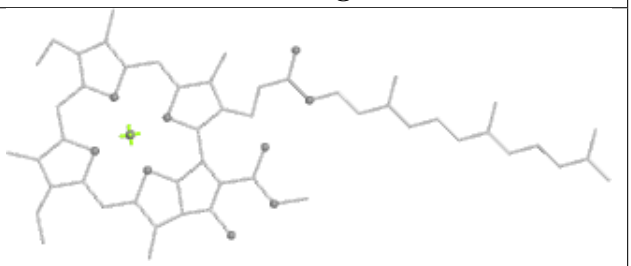
Ligand CHL G 609



Ligand CLA s 603



Ligand CLA 7 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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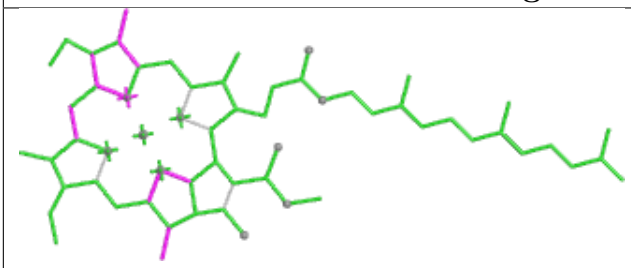
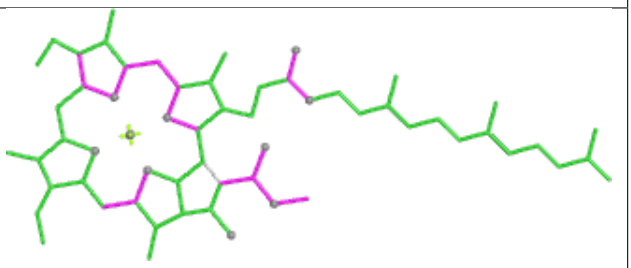
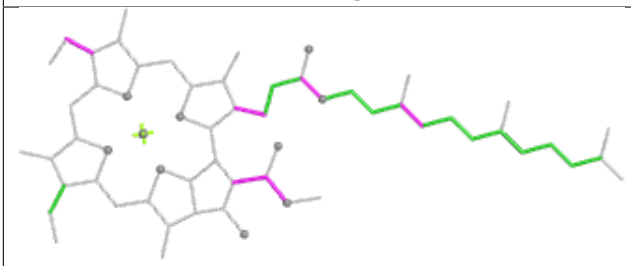
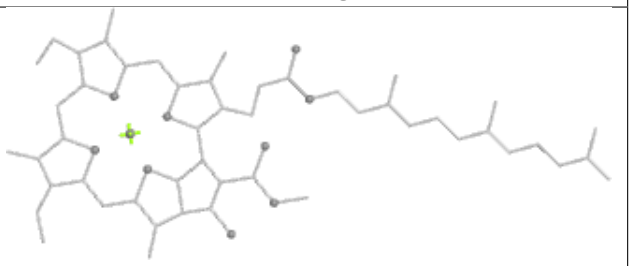
 Bond lengths	 Bond angles
 Torsions	 Rings

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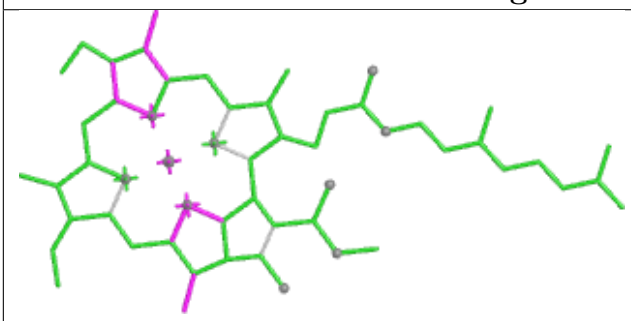
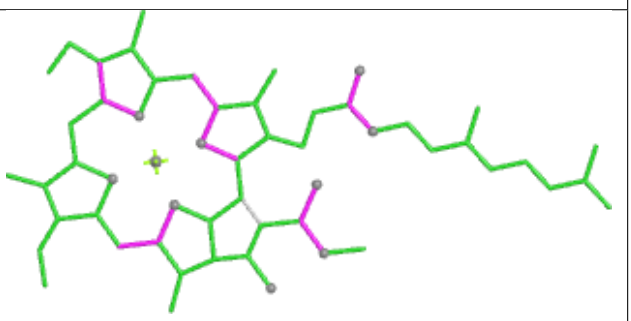
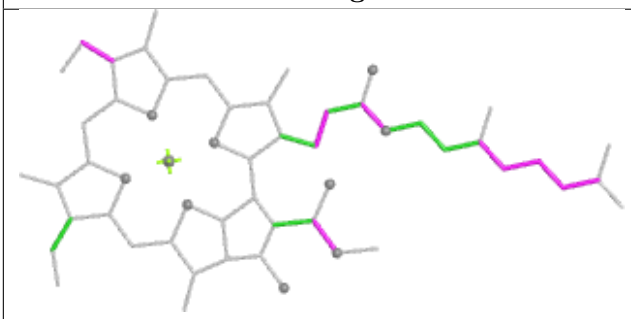
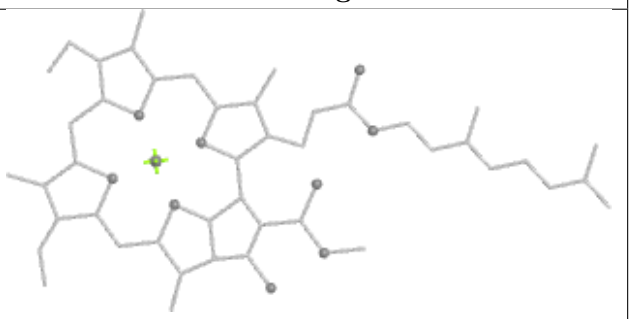
 Bond lengths	 Bond angles
 Torsions	 Rings

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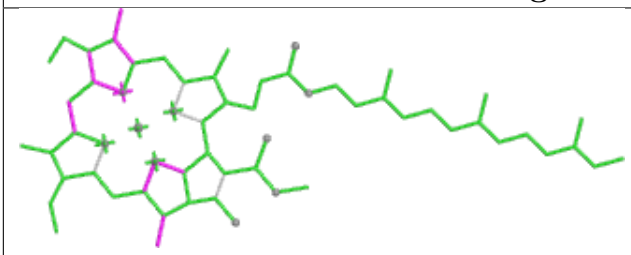
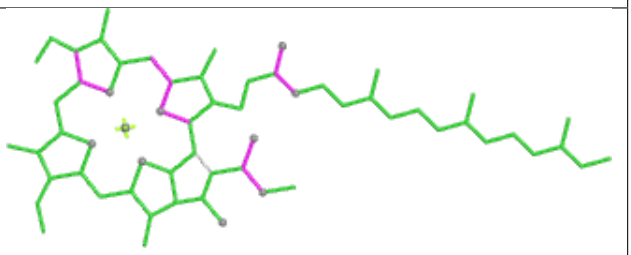
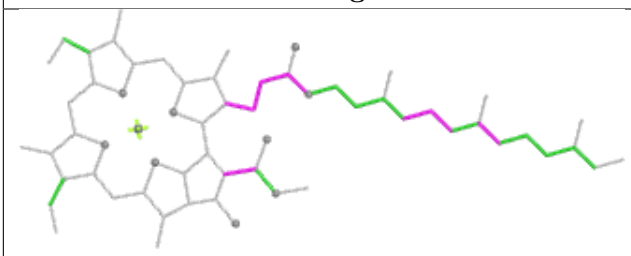
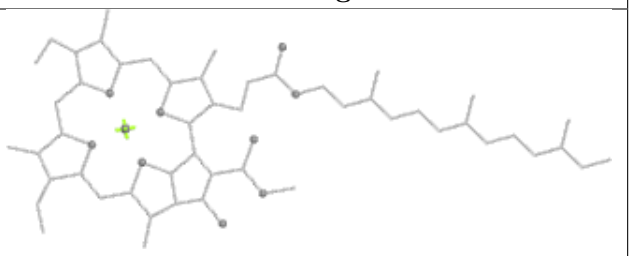
 Bond lengths	 Bond angles
 Torsions	 Rings

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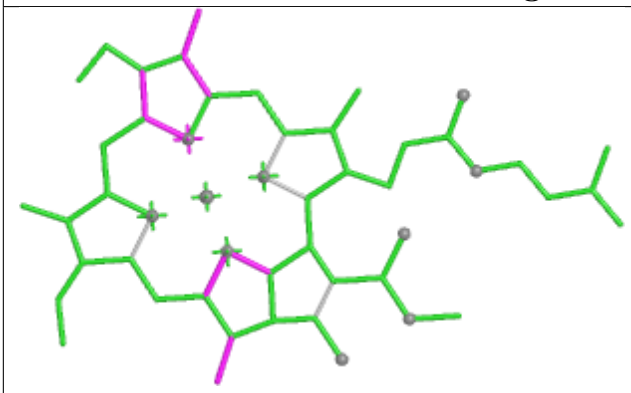
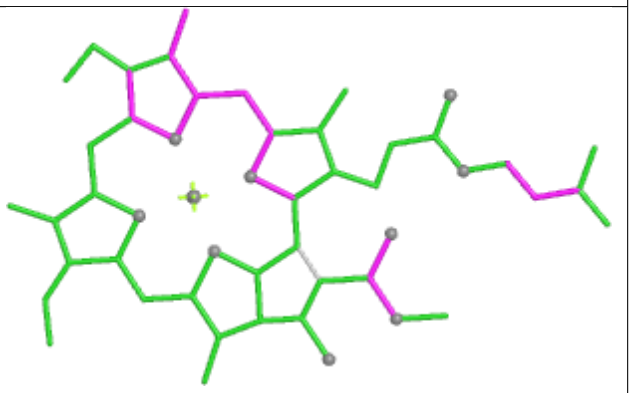
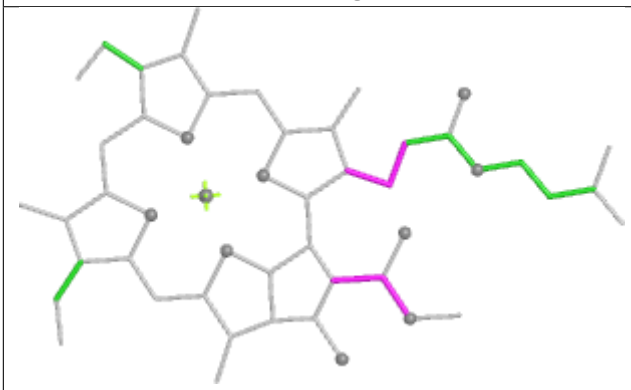
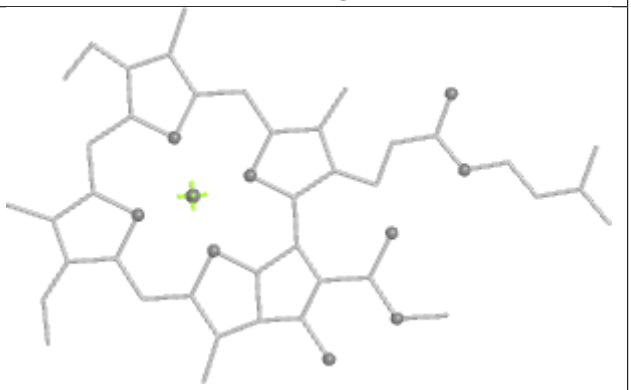
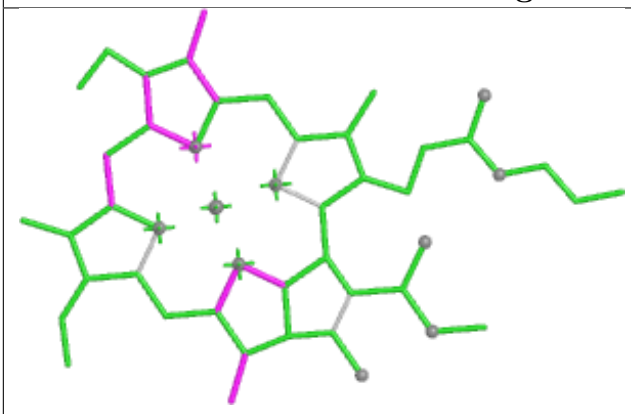
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Ba 315



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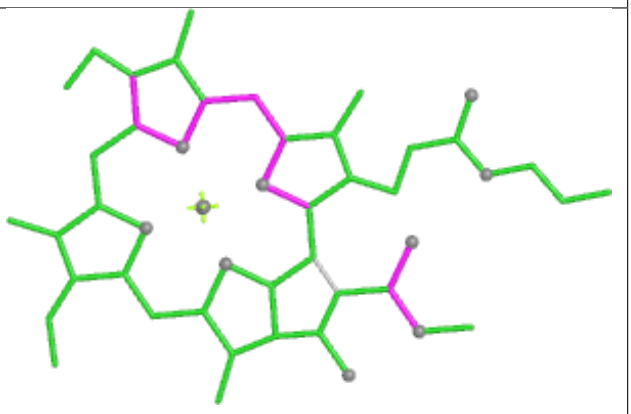

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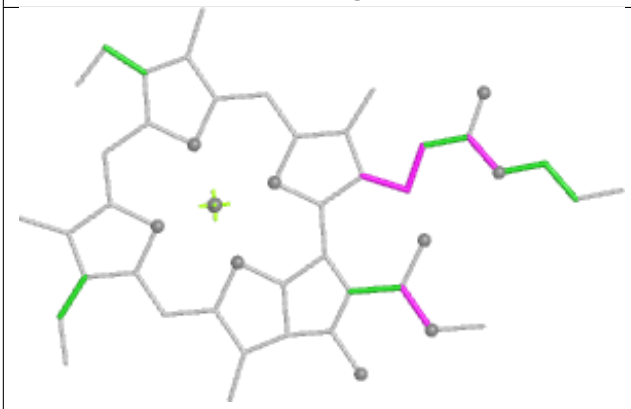

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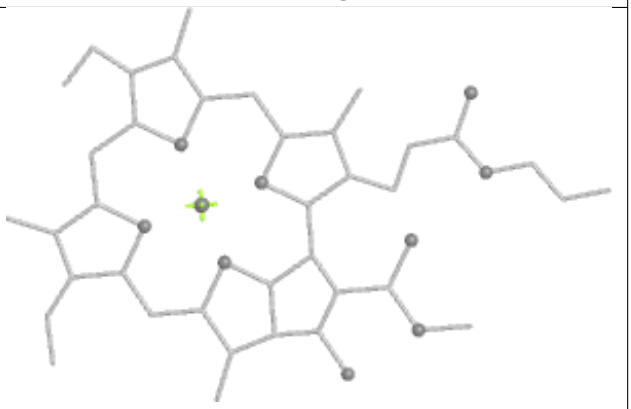
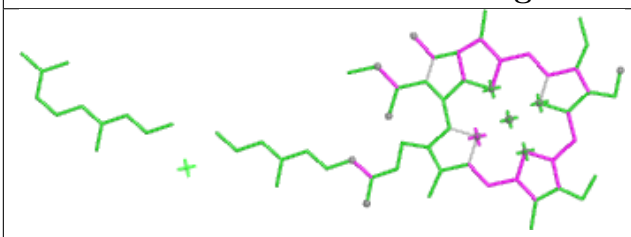


Rings

Ligand CHL A2 601



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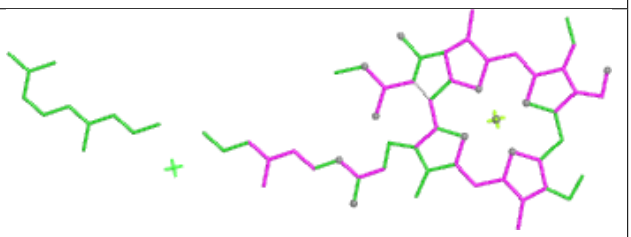

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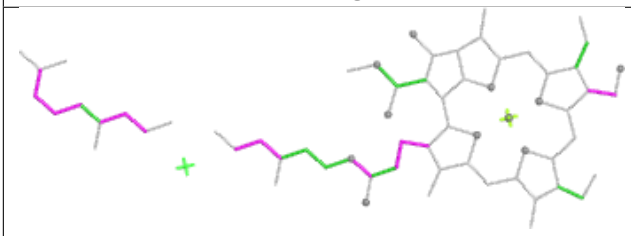

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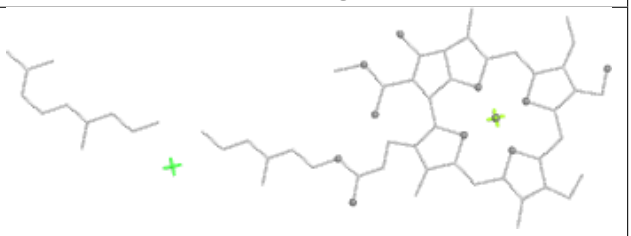

Rings

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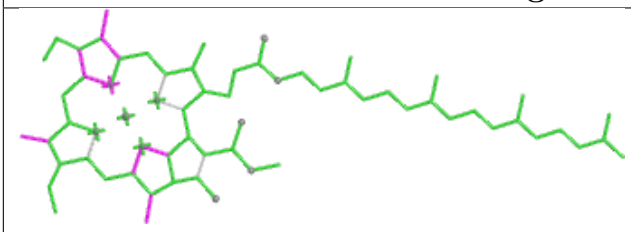
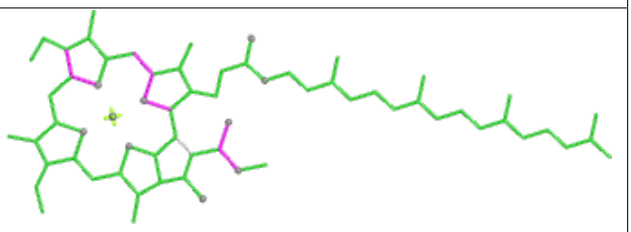
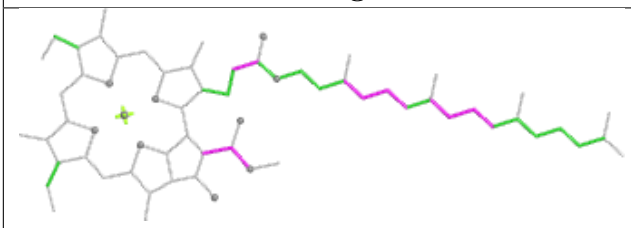
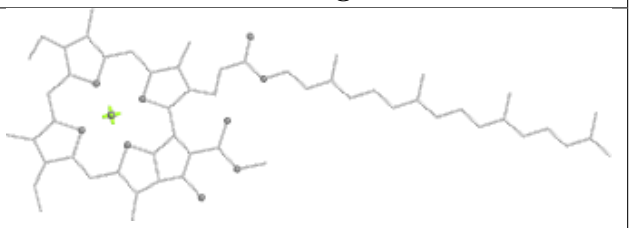
 Bond lengths	 Bond angles
 Torsions	 Rings

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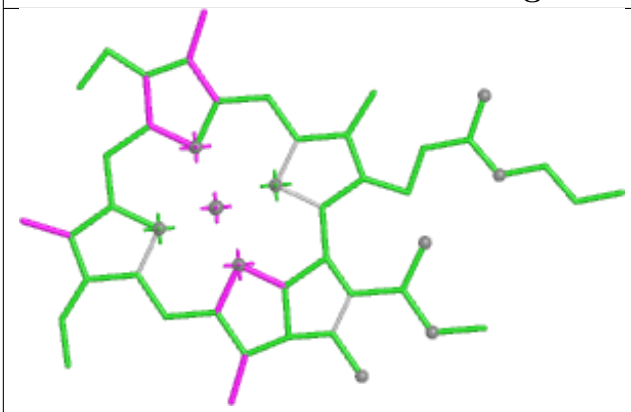
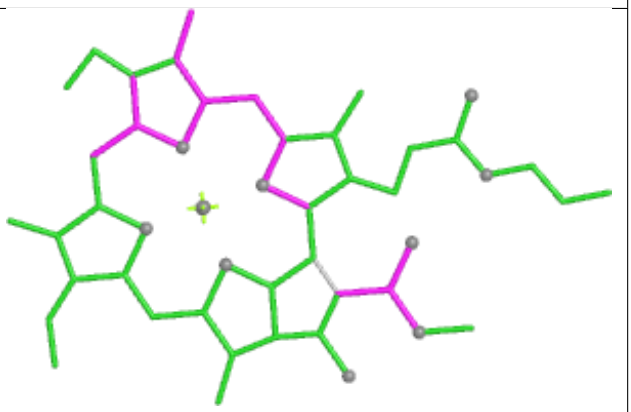
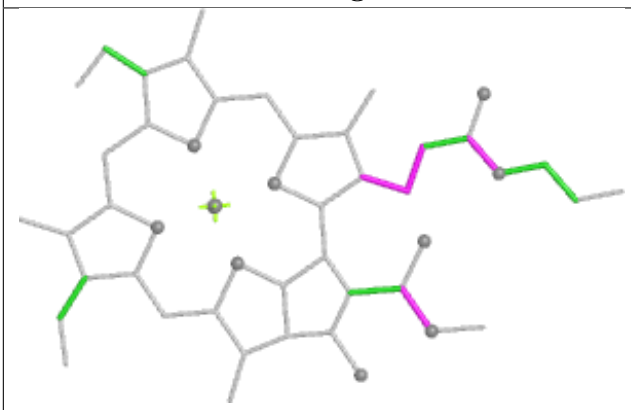
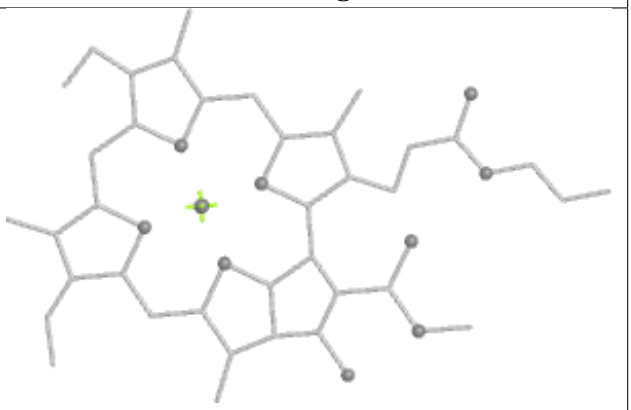
 Bond lengths	 Bond angles
 Torsions	 Rings

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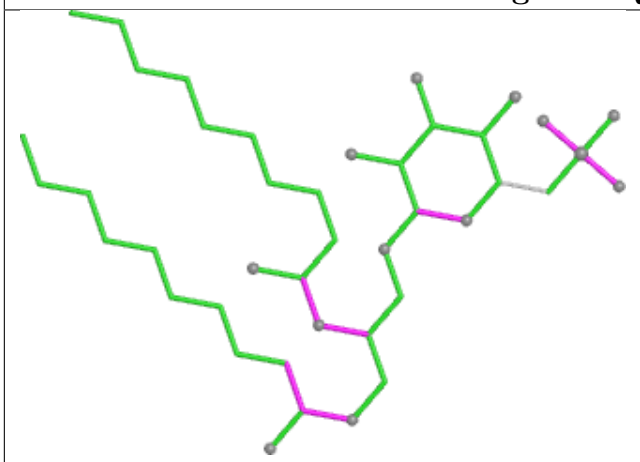
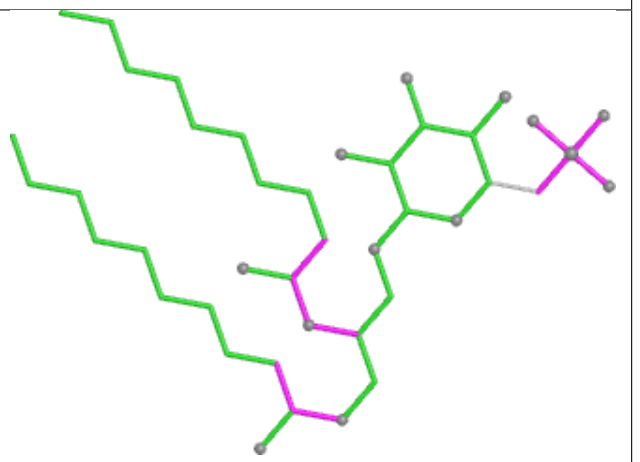
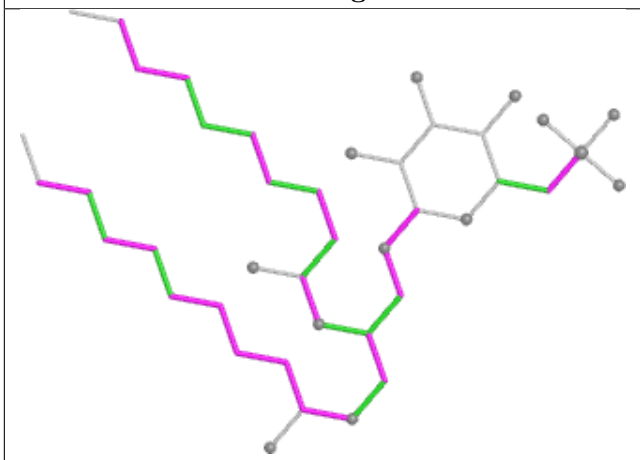
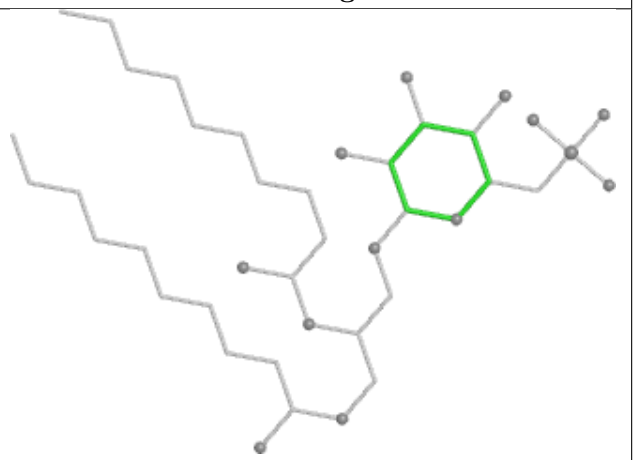
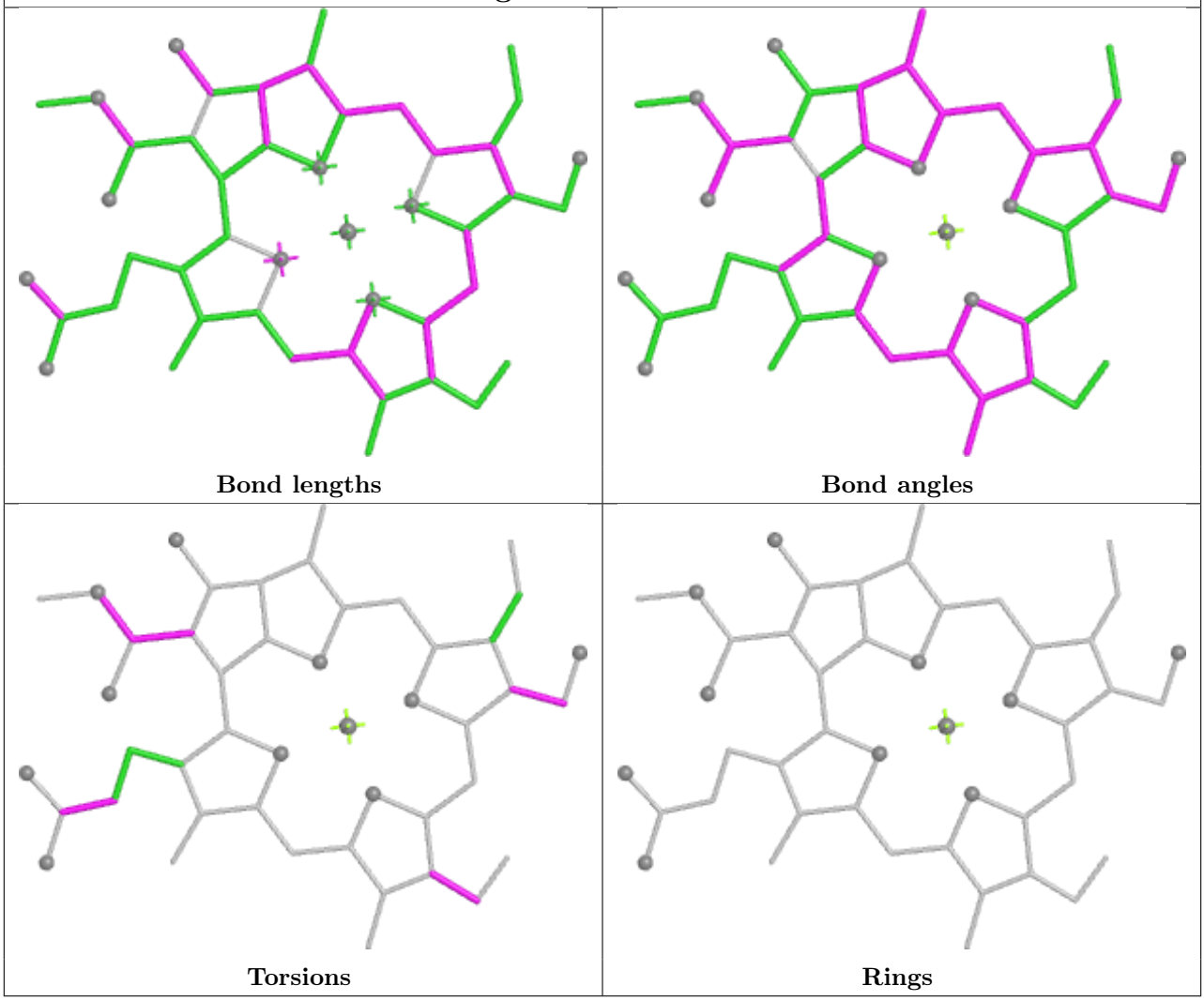
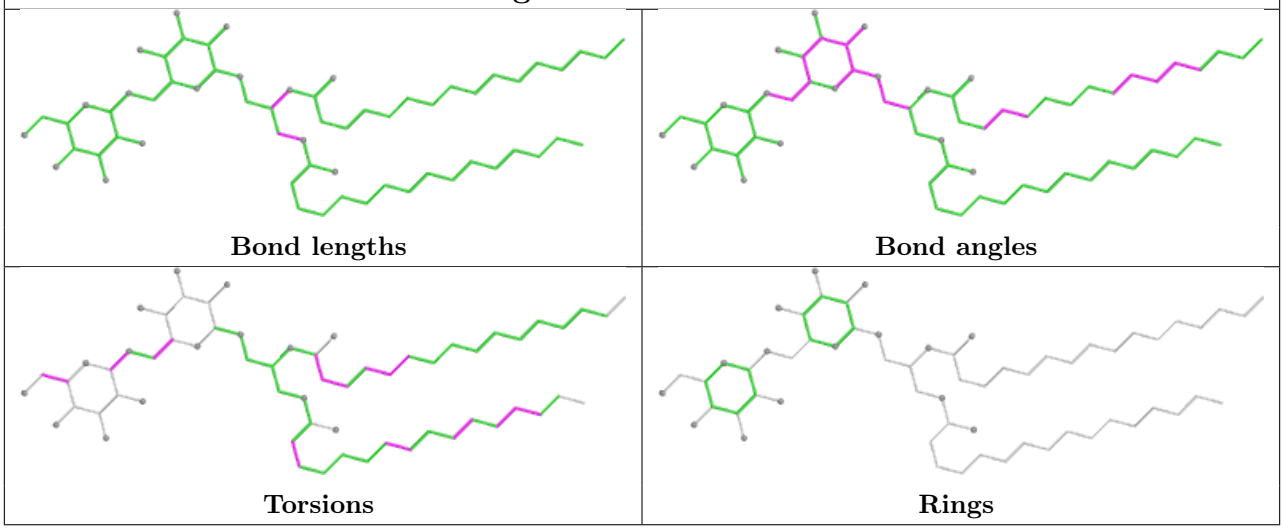
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL S 605



Ligand DGD Av 102



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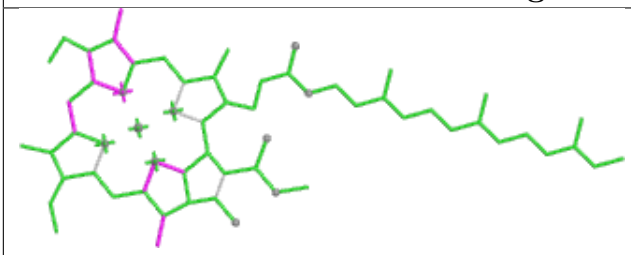

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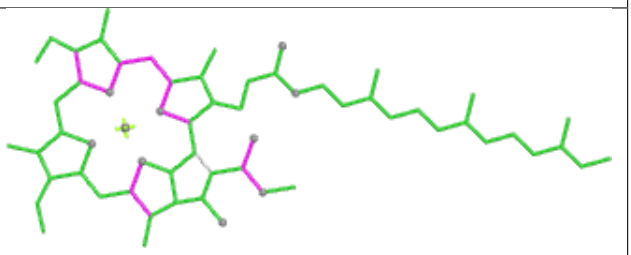
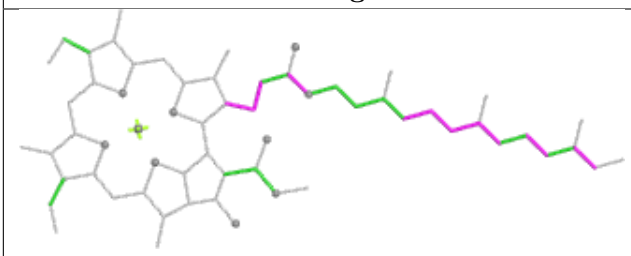
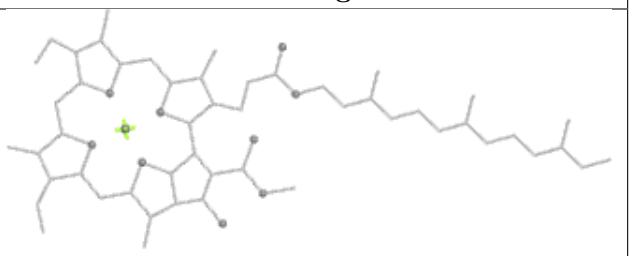


Bond angles

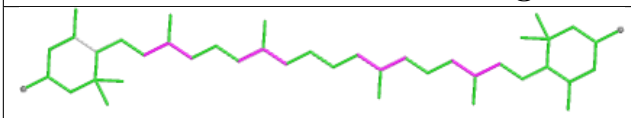


Torsions



Rings

Ligand LUT BJ 615



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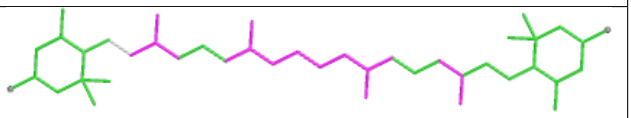
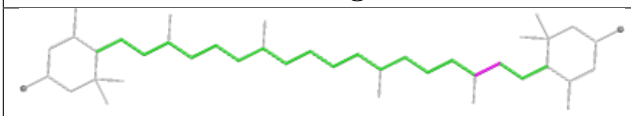


Bond angles



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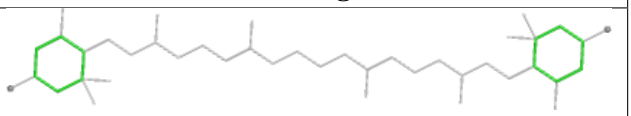
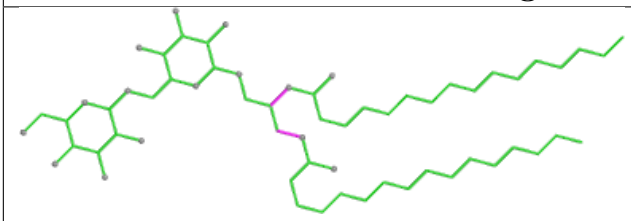


Rings

Ligand DGD H 102



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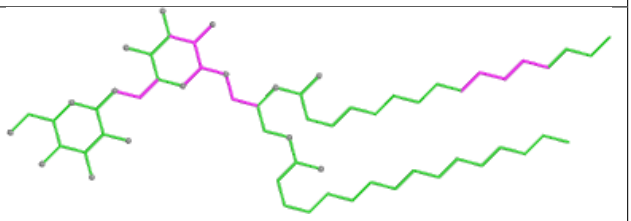
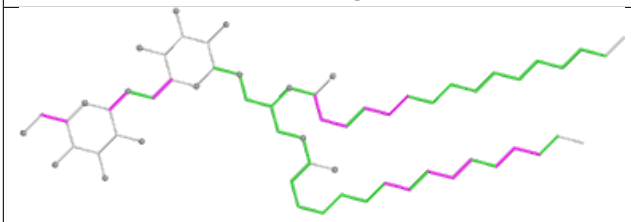


Bond angles



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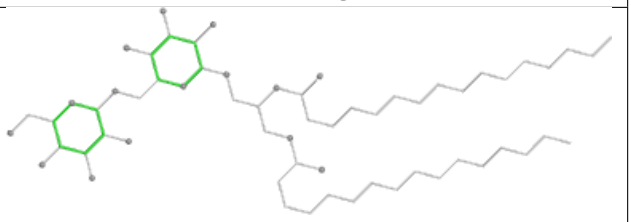
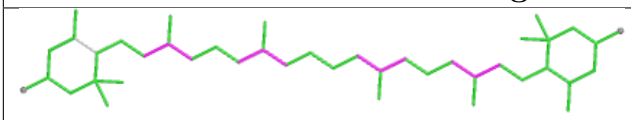
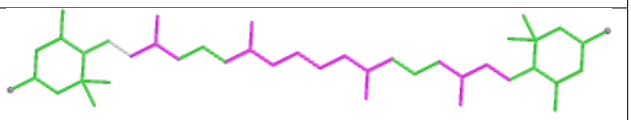


Rings

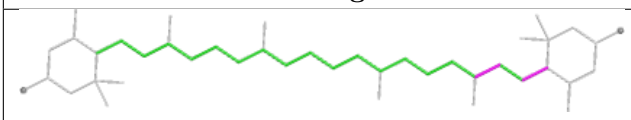
Ligand LUT AA 316



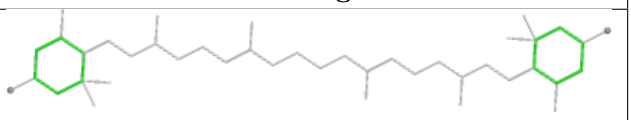
Bond lengths



Bond angles

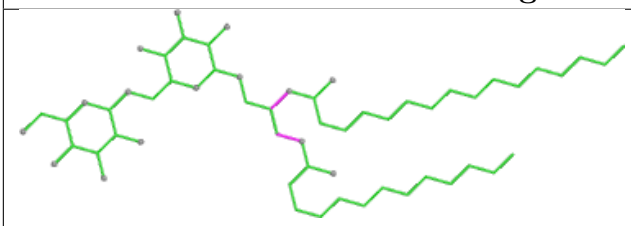


Torsions

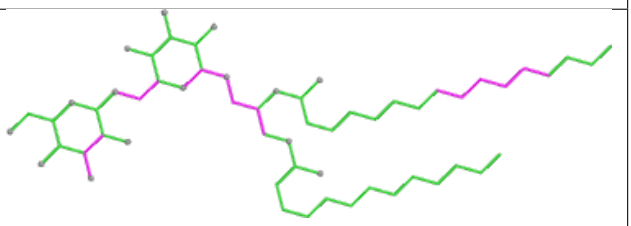


Rings

Ligand DGD A 402



Bond lengths



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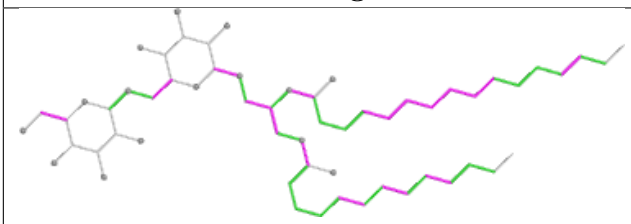

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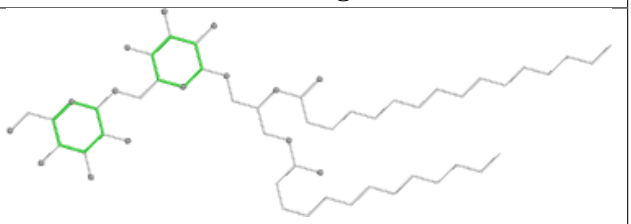
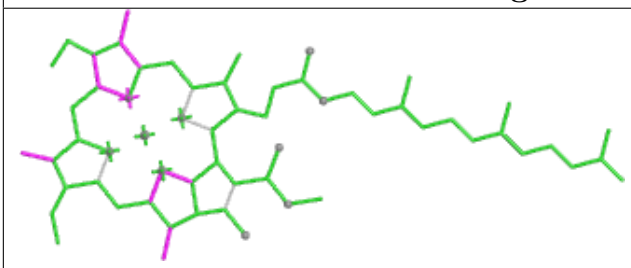


Rings

Ligand CLA BD 410



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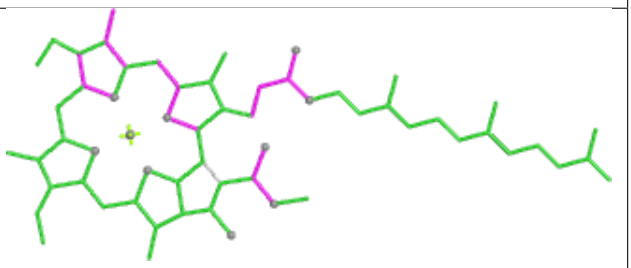

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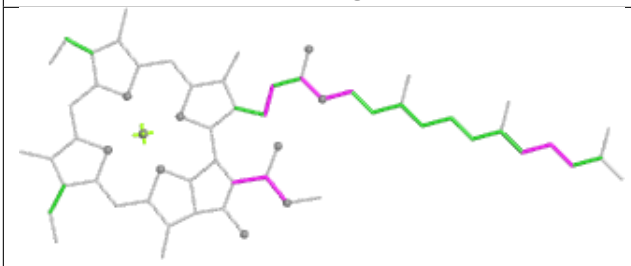

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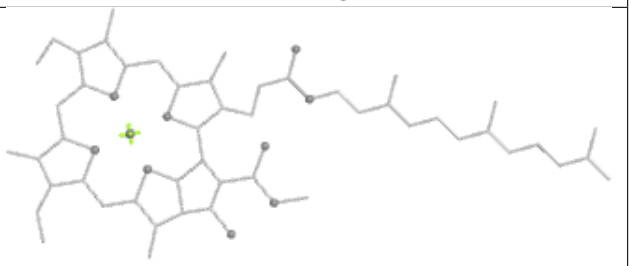

Rings

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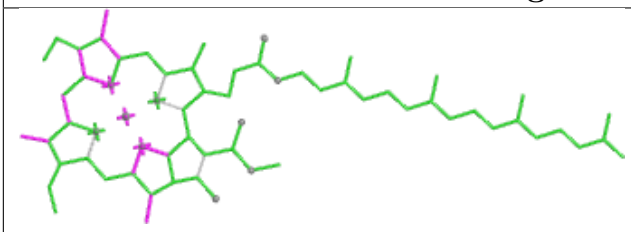
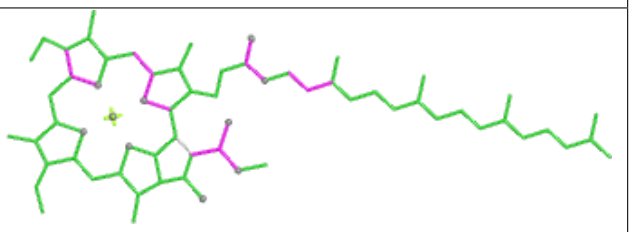
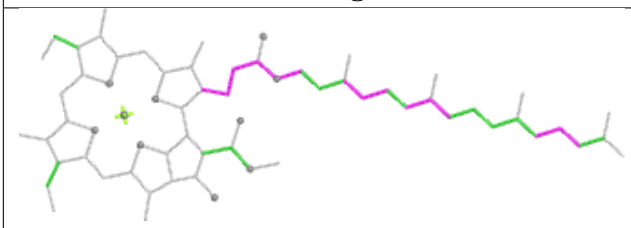
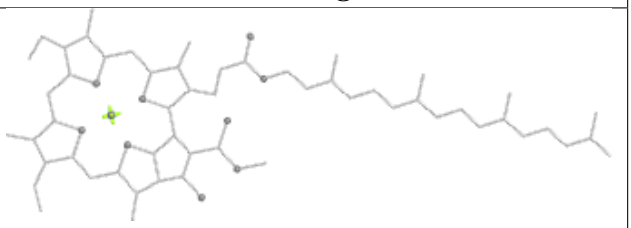
 Bond lengths	 Bond angles
 Torsions	 Rings

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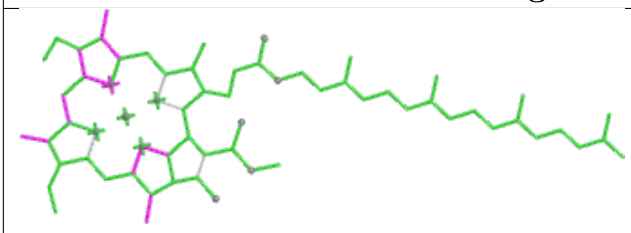
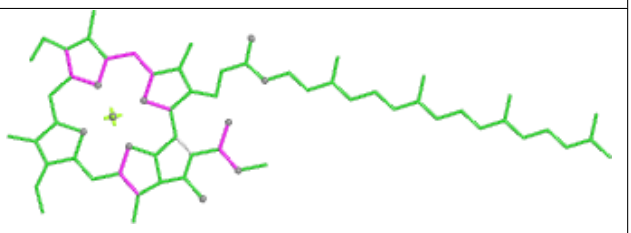
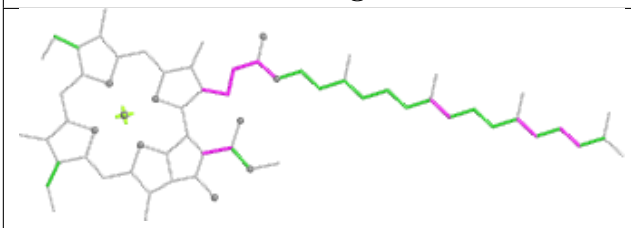
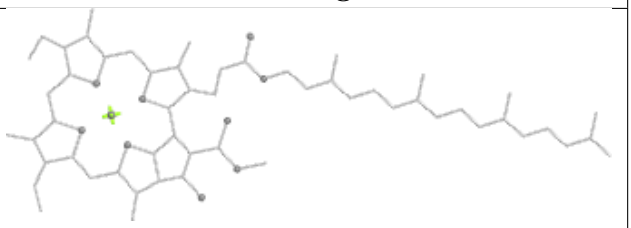
 Bond lengths	 Bond angles
 Torsions	 Rings

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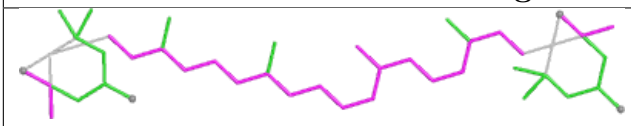
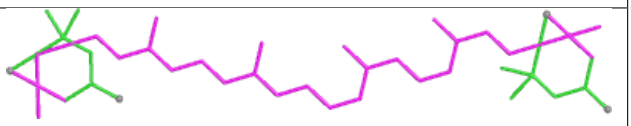
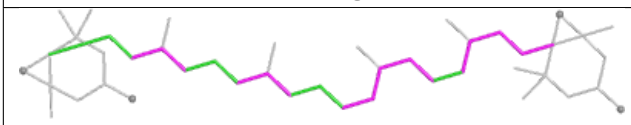
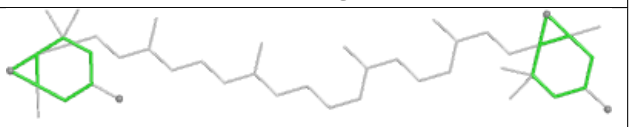
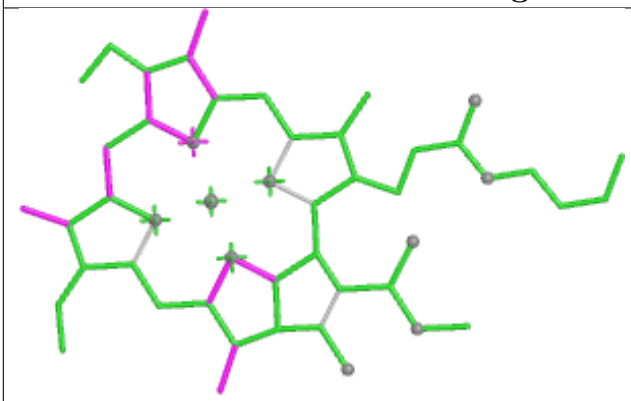
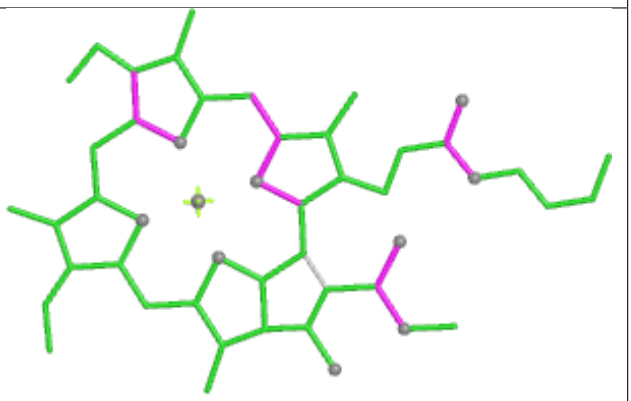
 Bond lengths	 Bond angles
 Torsions	 Rings

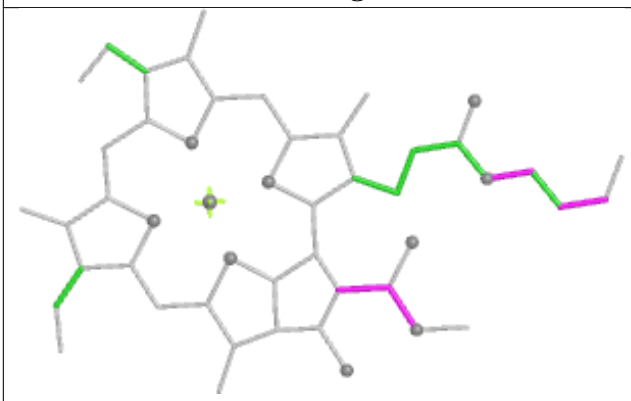
Ligand CLA BV 611



Bond lengths



Bond angles



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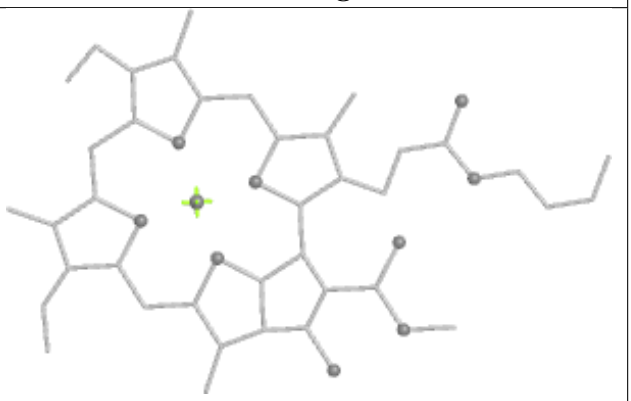
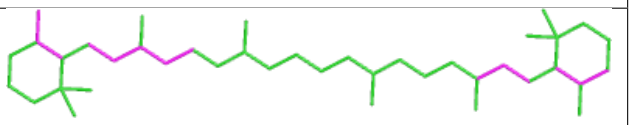


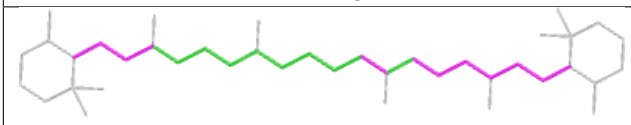
Rings

Ligand BCR B 623

Bond lengths



Bond angles



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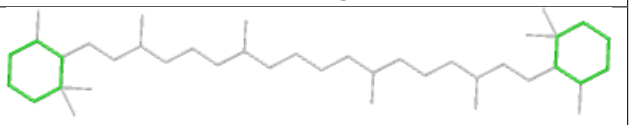
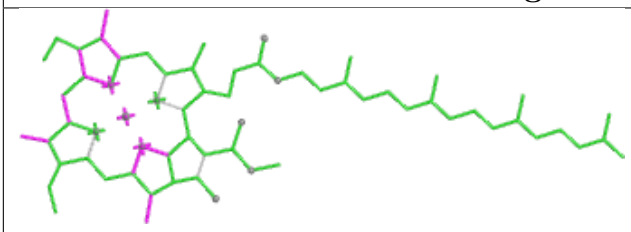


Rings

Ligand CLA C 512



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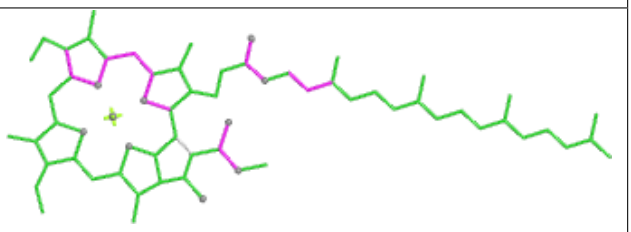

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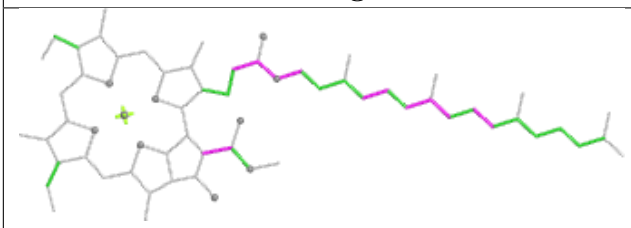

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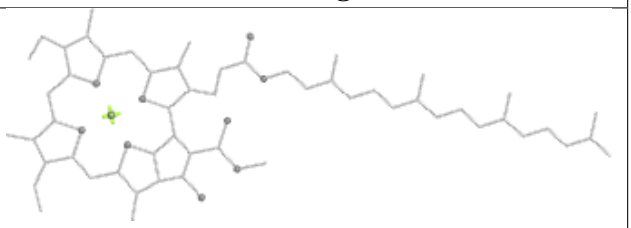
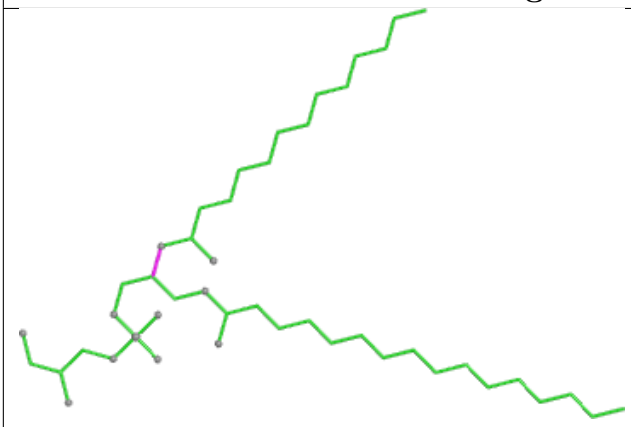


Rings

Ligand LHG b 623



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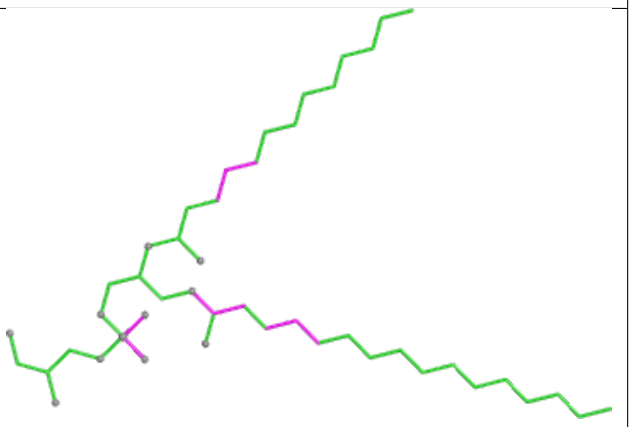

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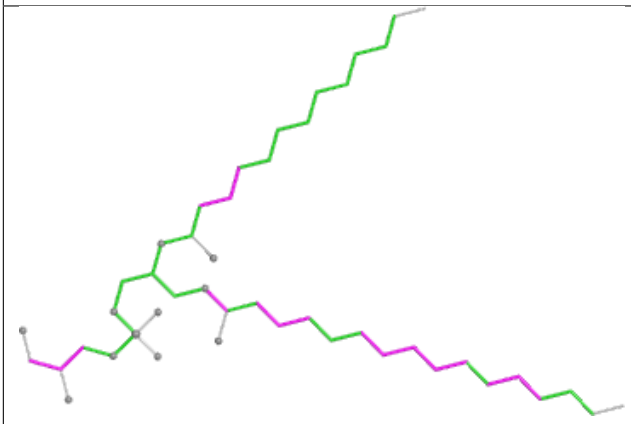

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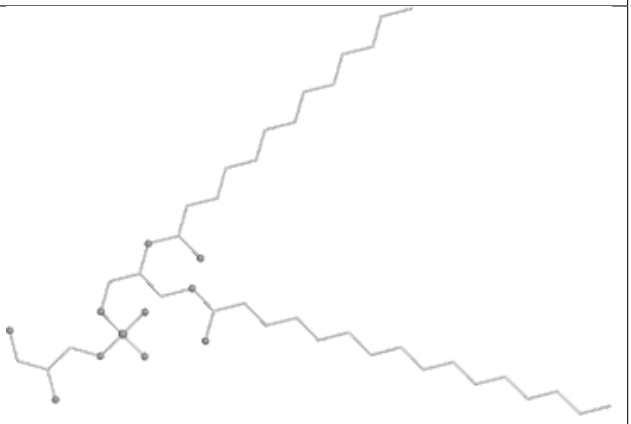
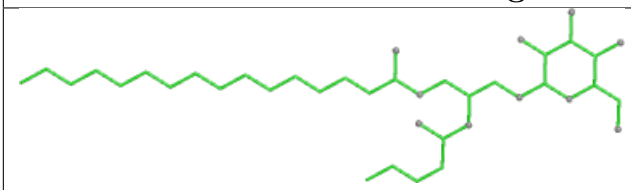
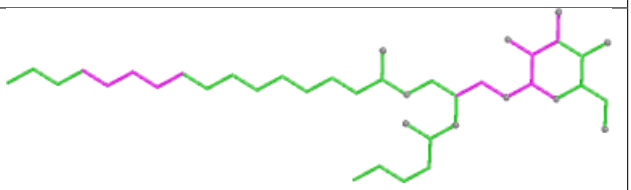
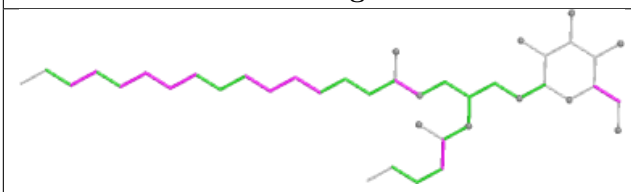
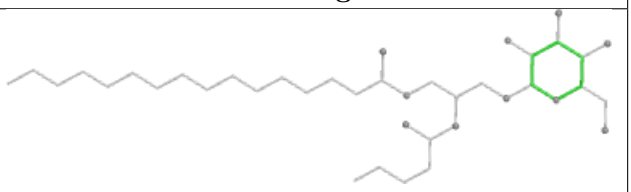


Rings

Ligand LMG Aw 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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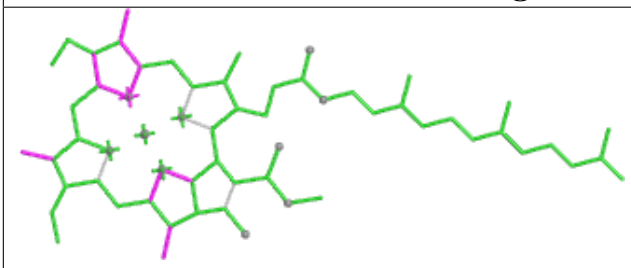
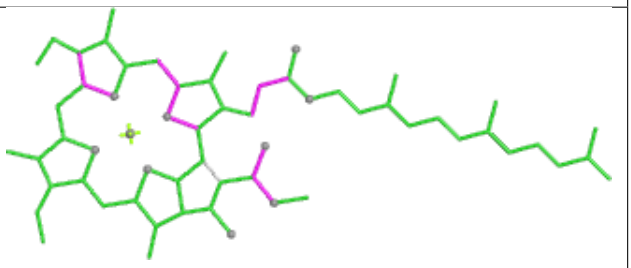
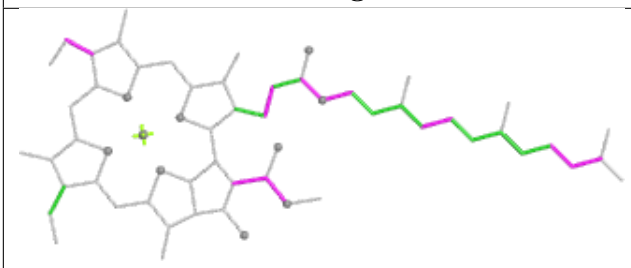
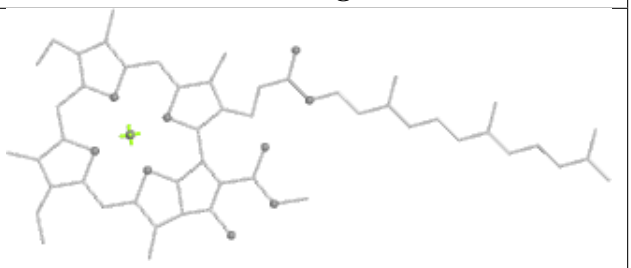
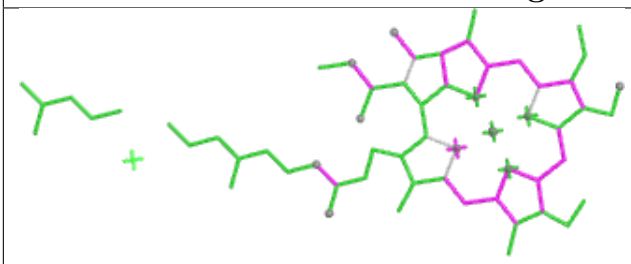
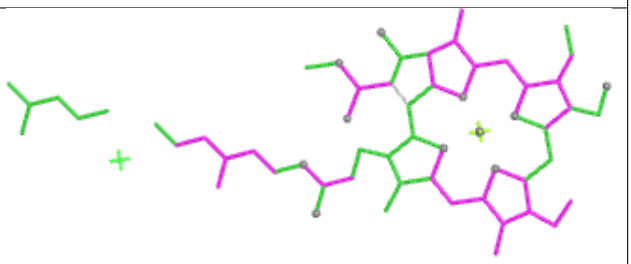
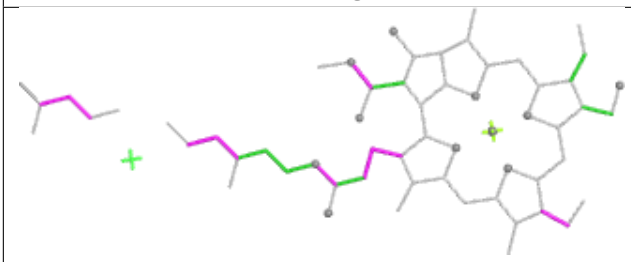
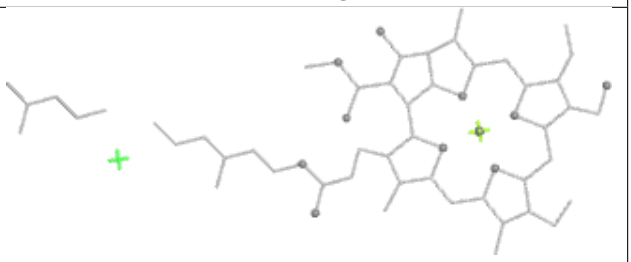
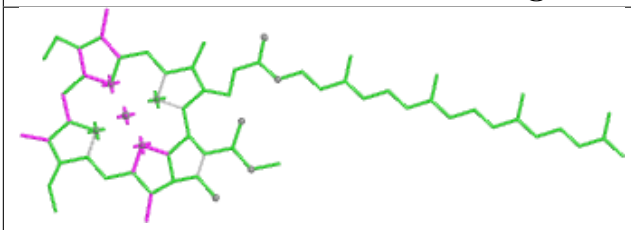
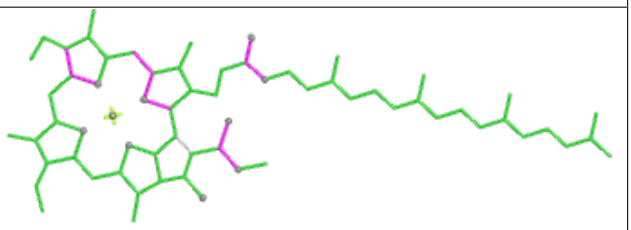
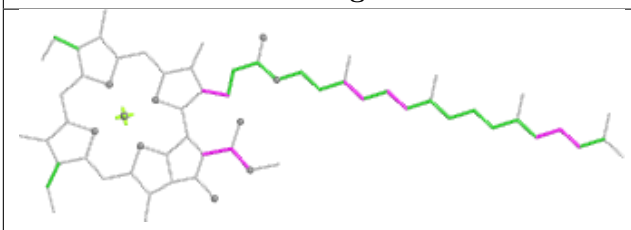
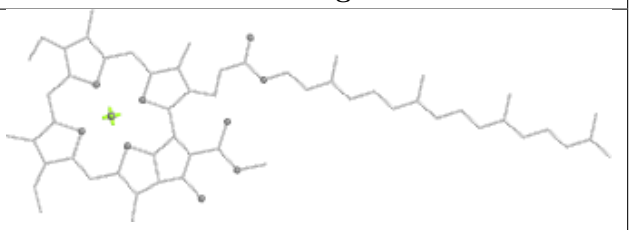
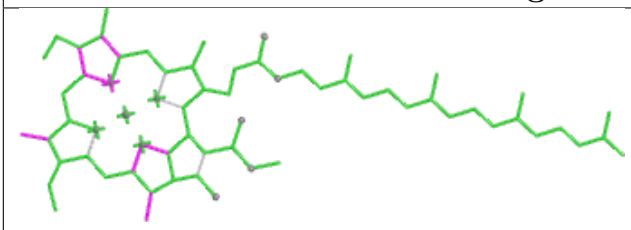
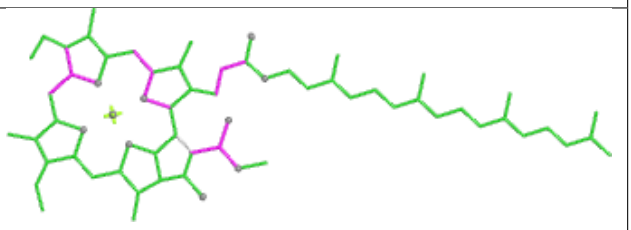
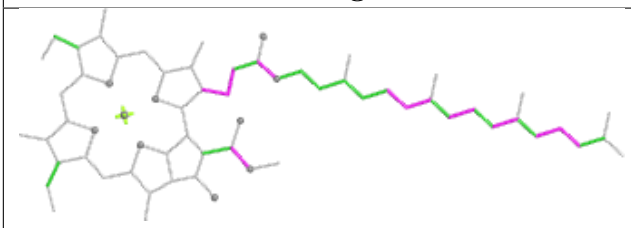
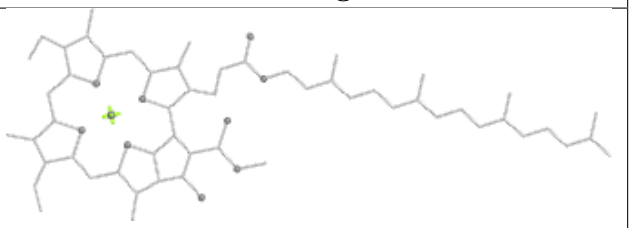
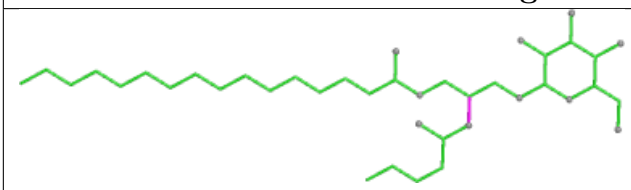
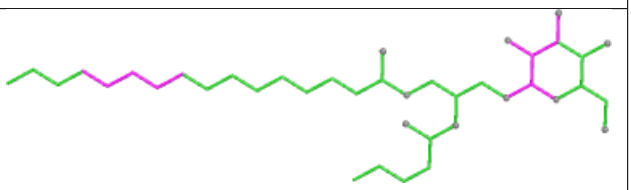
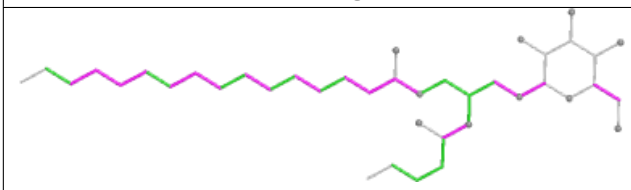
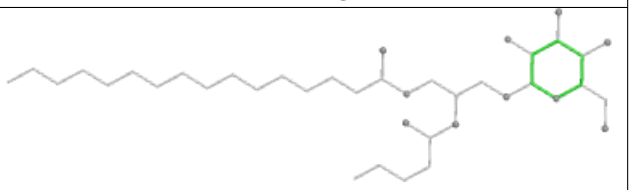
 Bond lengths	 Bond angles
 Torsions	 Rings

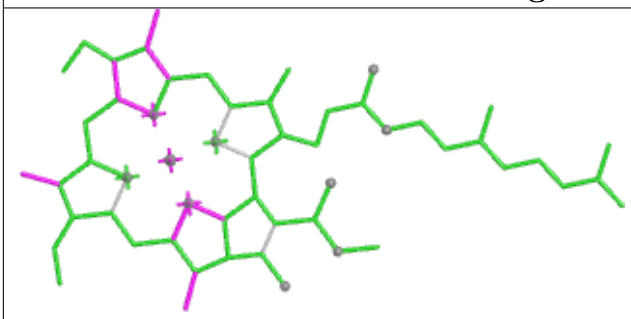
Ligand CHL 7 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 603



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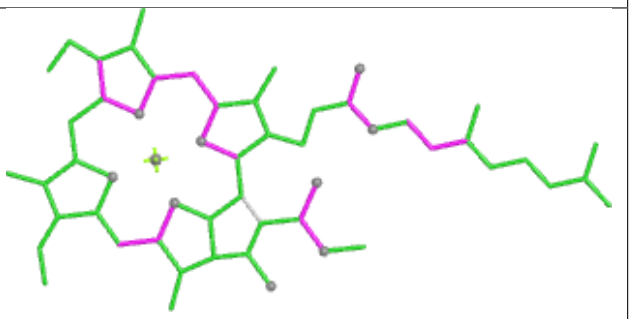

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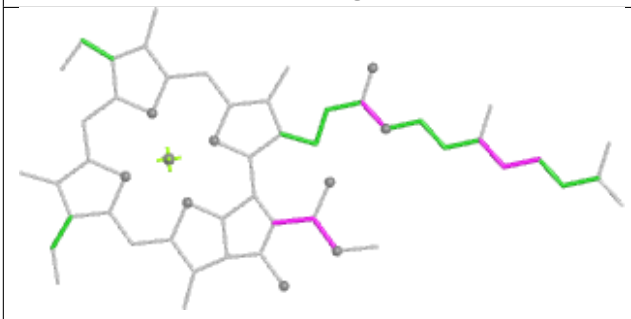

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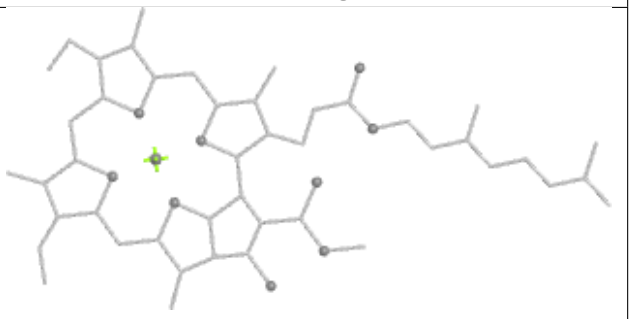
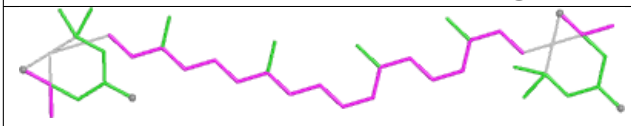


Rings

Ligand XAT BQ 619



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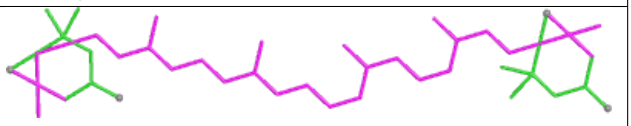

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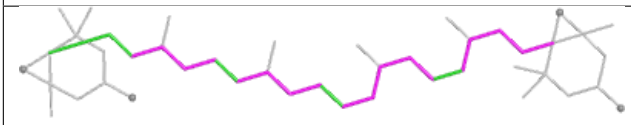

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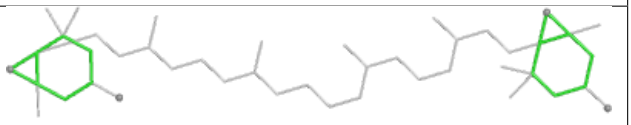
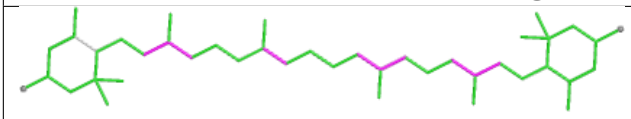


Rings

Ligand LUT 6 616



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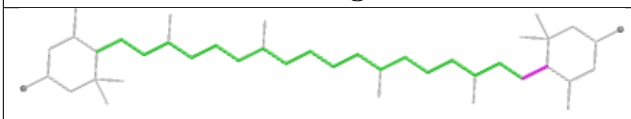

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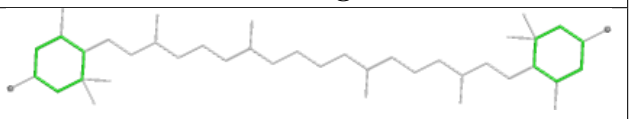
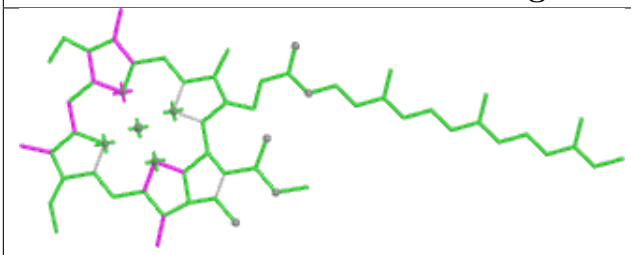
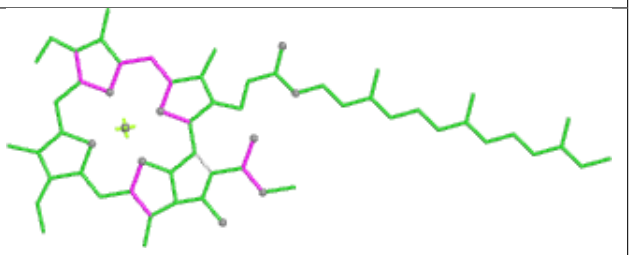
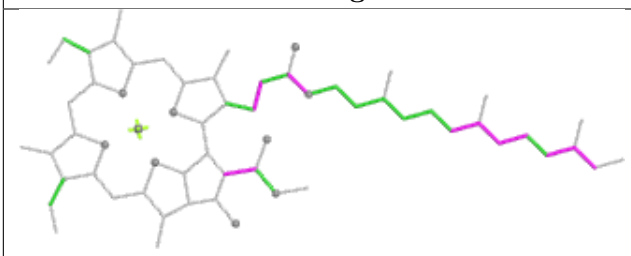
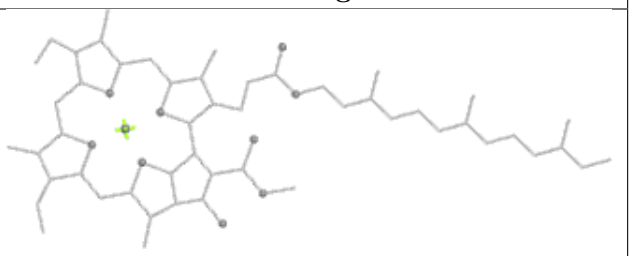


Rings

Ligand CLA 9 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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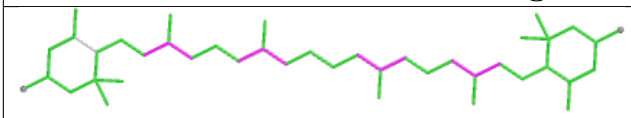
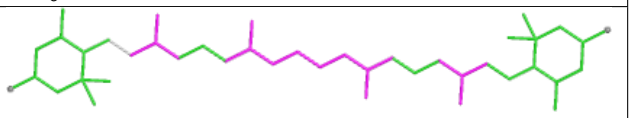
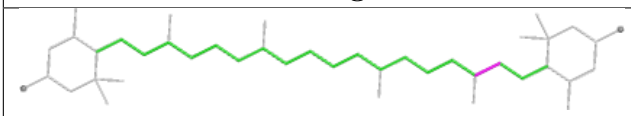
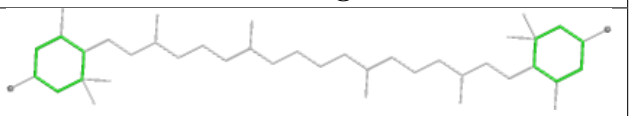
 Bond lengths	 Bond angles
 Torsions	 Rings

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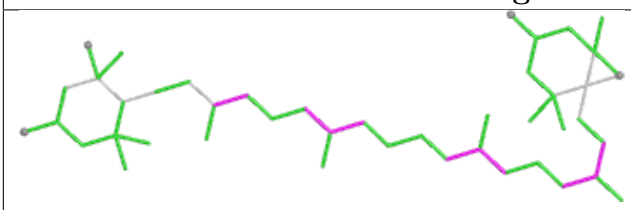
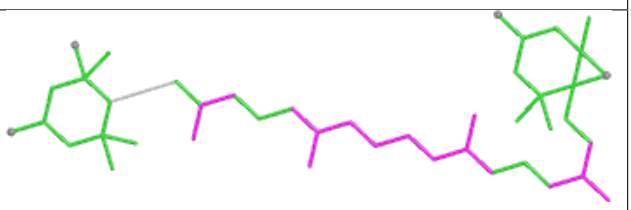
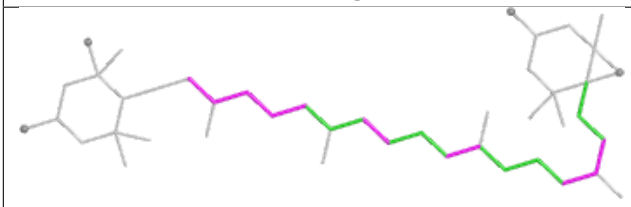
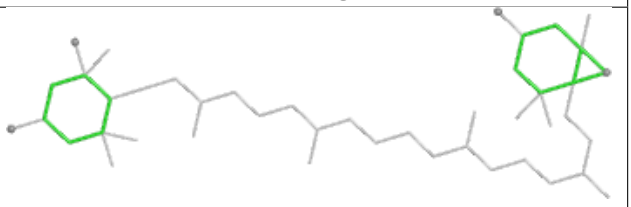
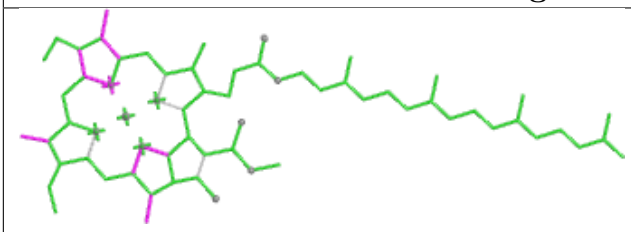
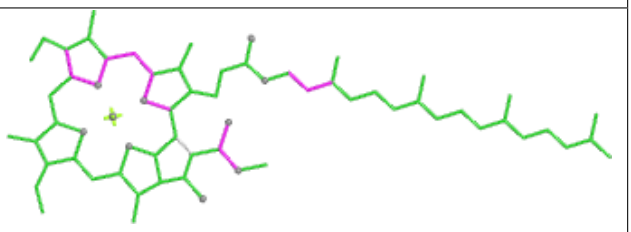
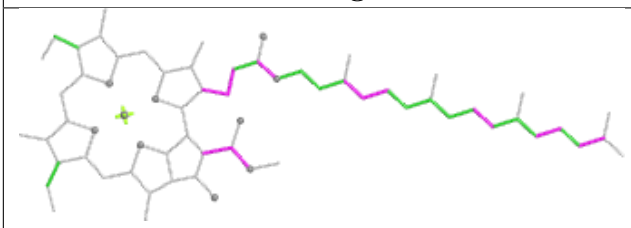
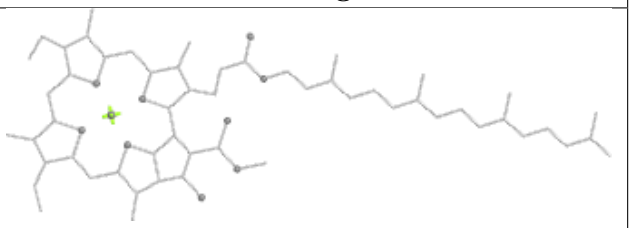
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

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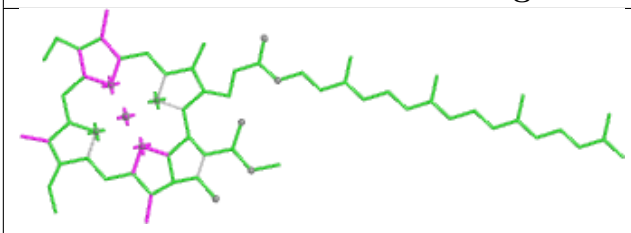
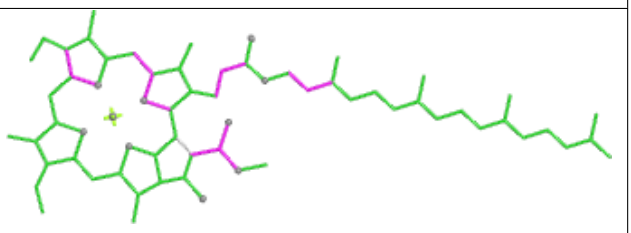
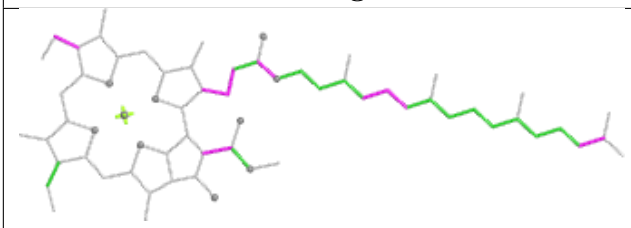
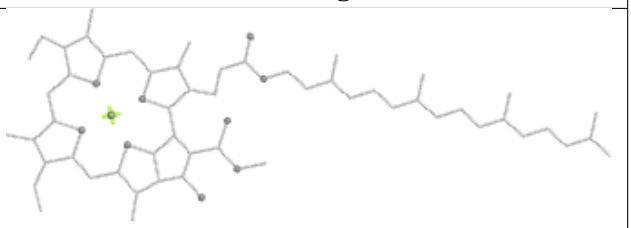
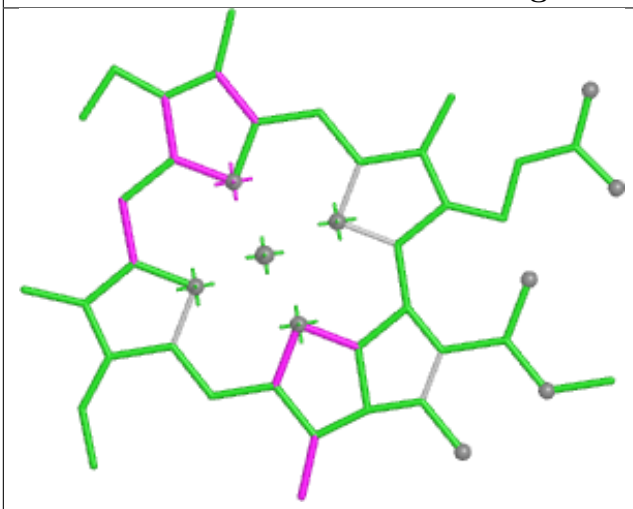
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 608



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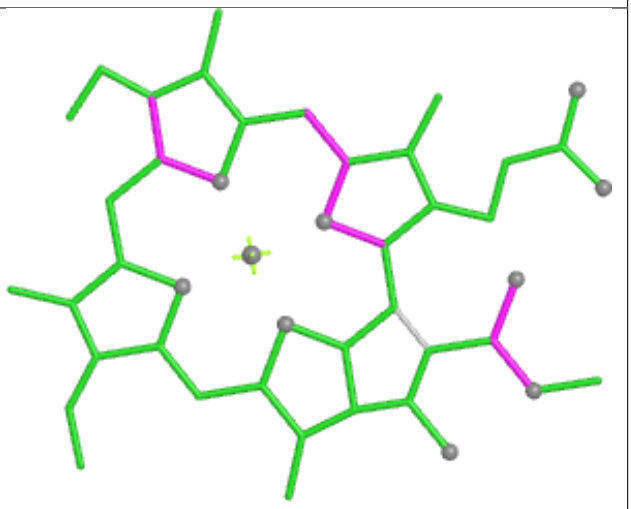

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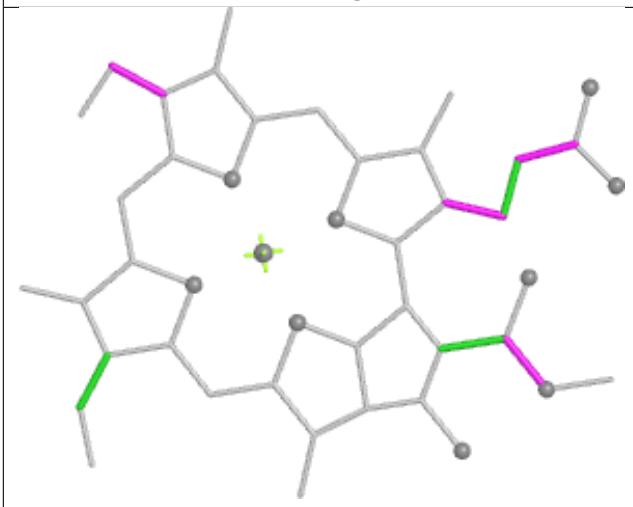
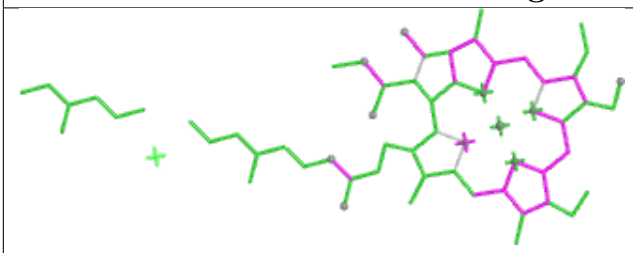


Torsions

Rings

Ligand CHL 5 609



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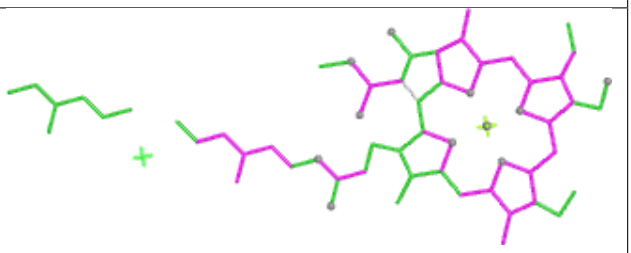

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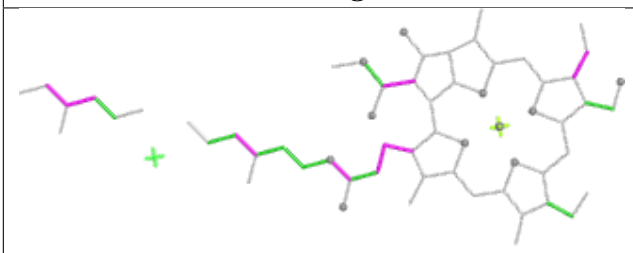

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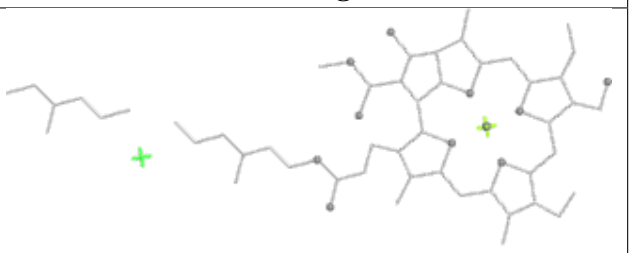
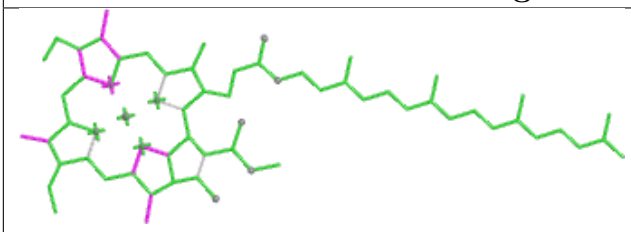


Rings

Ligand CLA BF 509



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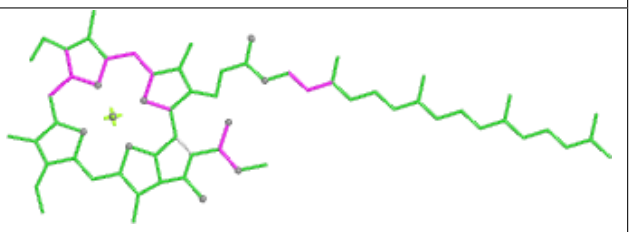

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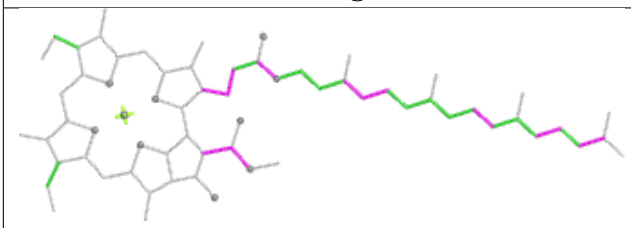

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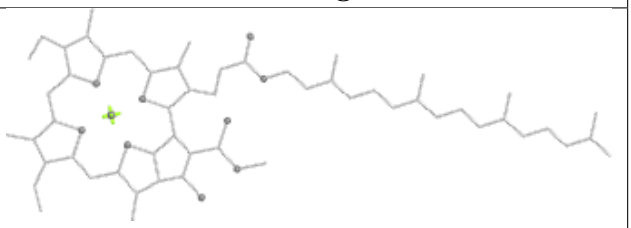
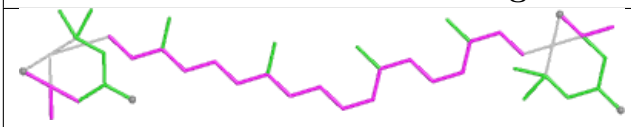


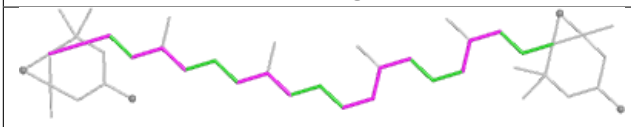
Rings

Ligand XAT AA 301



Bond lengths

Bond angles



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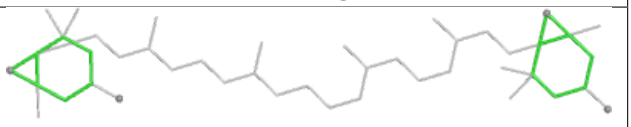
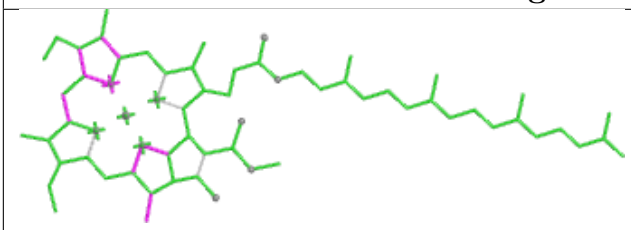
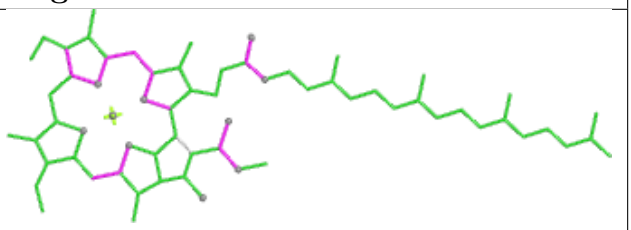


Rings

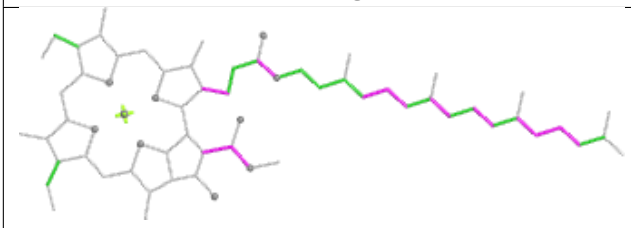
Ligand CLA g 602



Bond lengths



Bond angles



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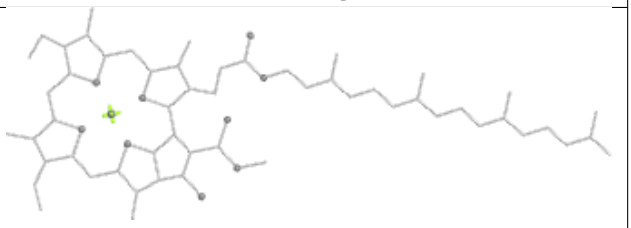
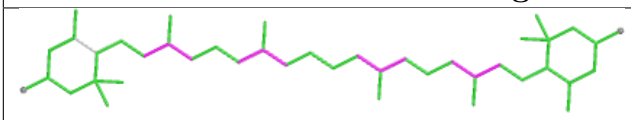
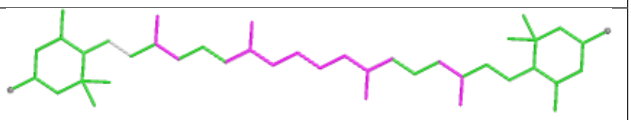
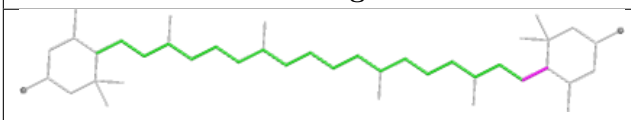
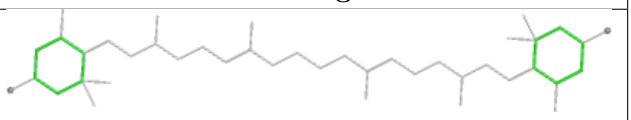


Rings

Ligand LUT BB 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

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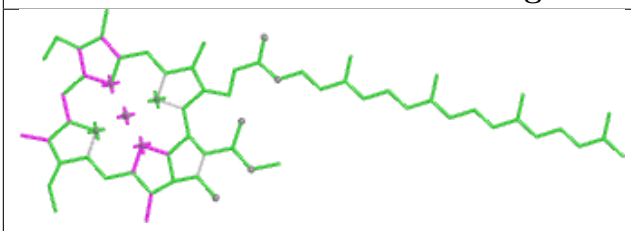
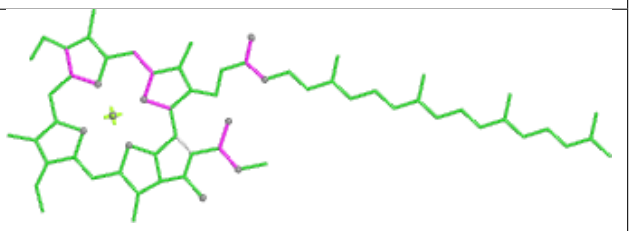
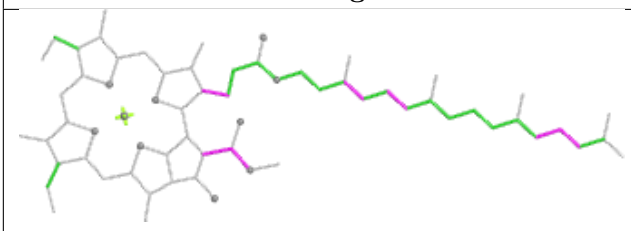
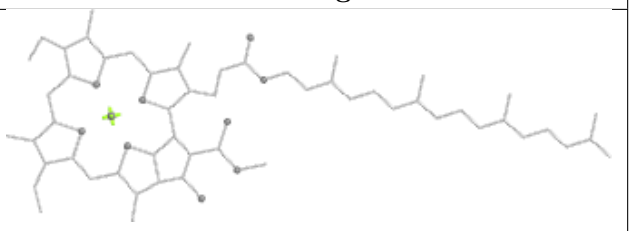
 Bond lengths	 Bond angles
 Torsions	 Rings

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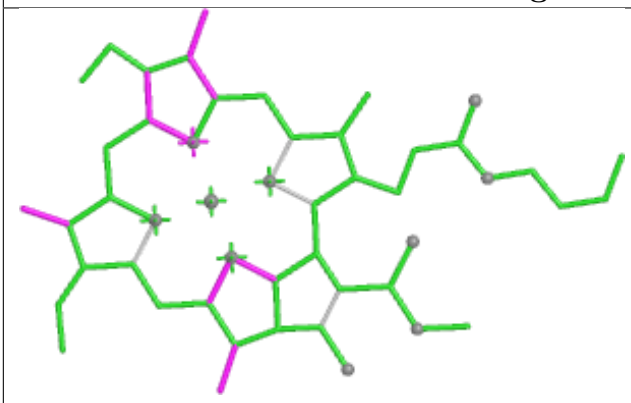
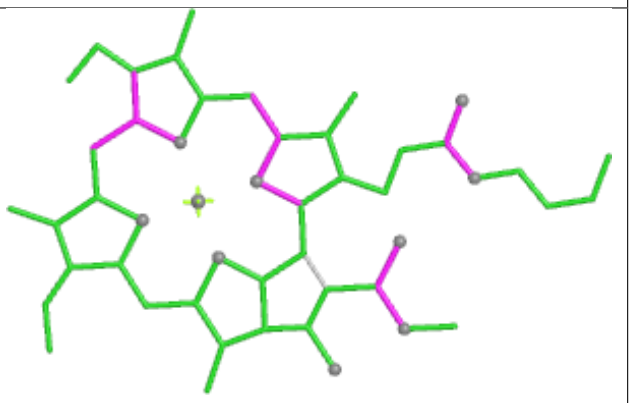
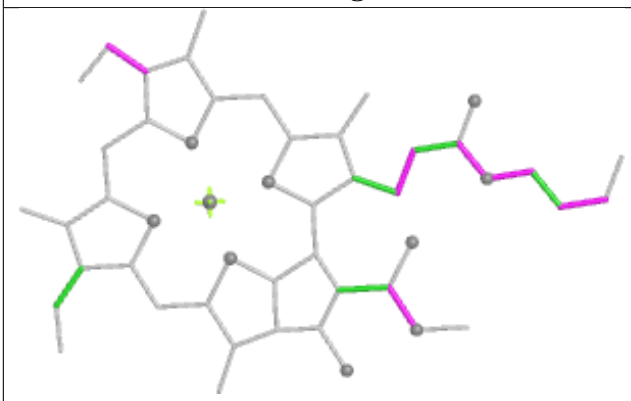
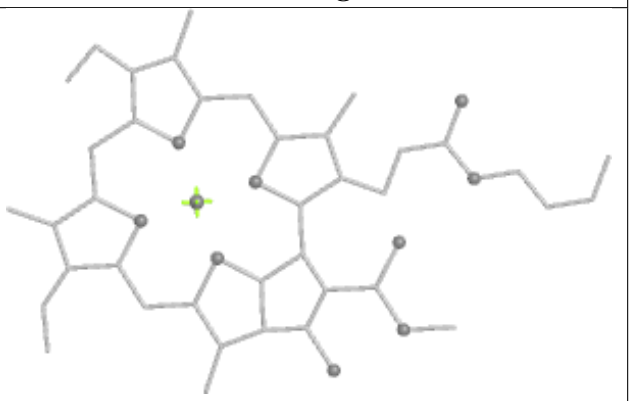
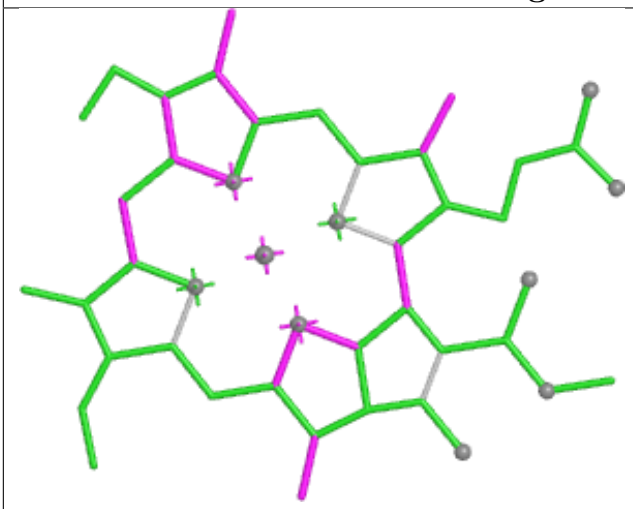
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 308



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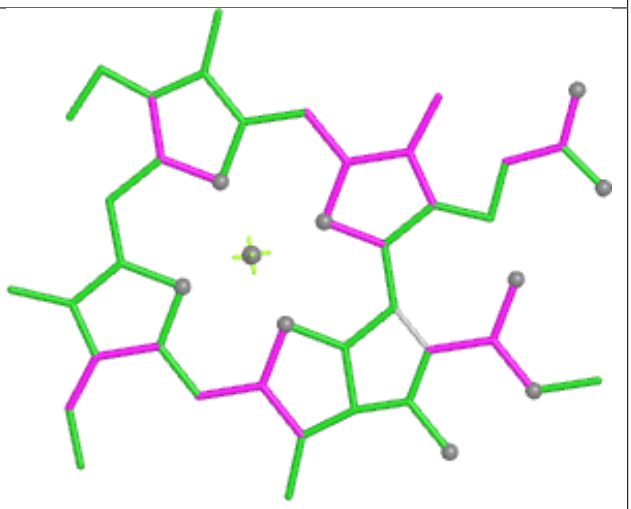
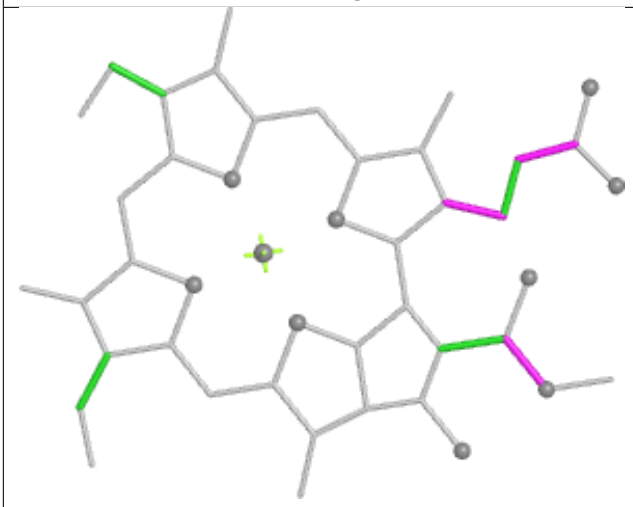


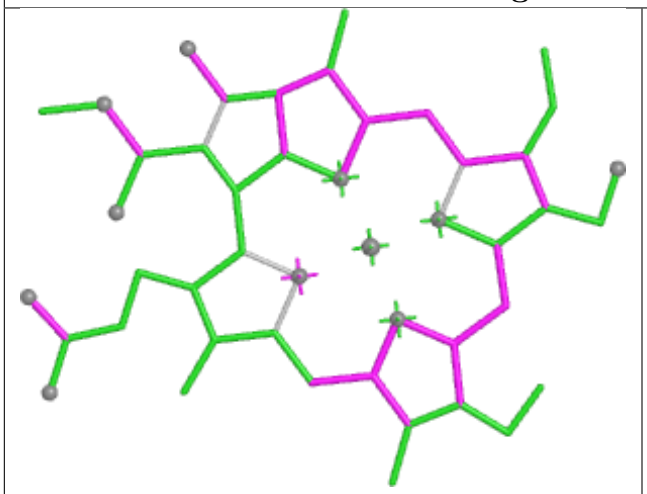
Bond angles



Torsions

Rings

Ligand CHL AB 307



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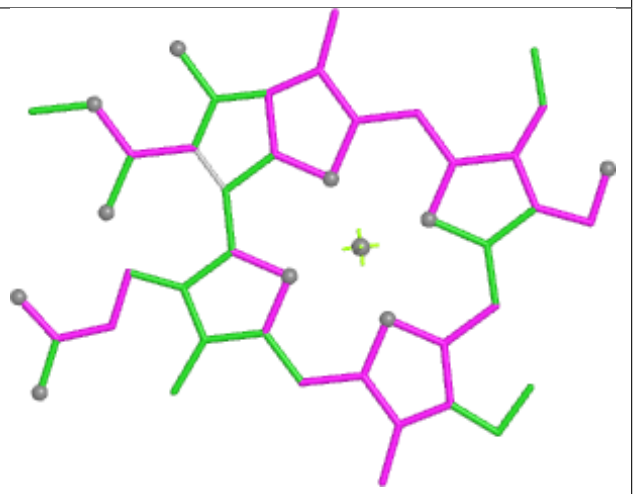

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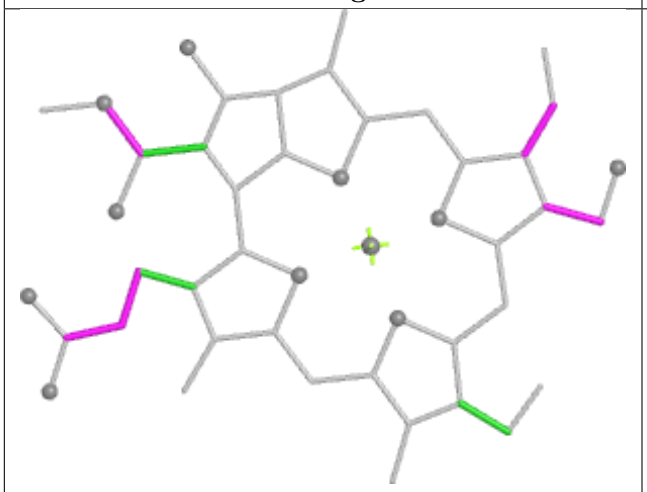

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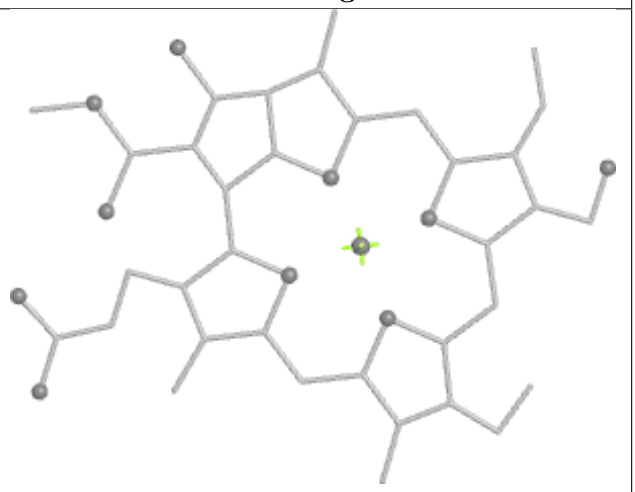
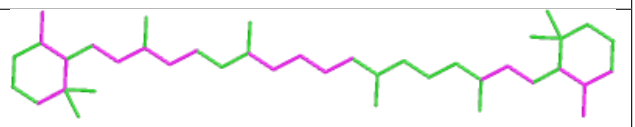


Rings

Ligand BCR H 101

Bond lengths



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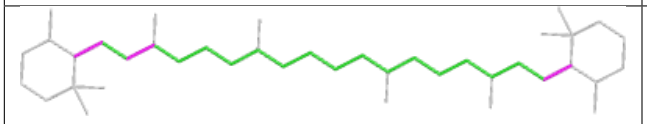

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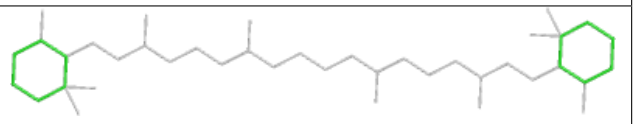
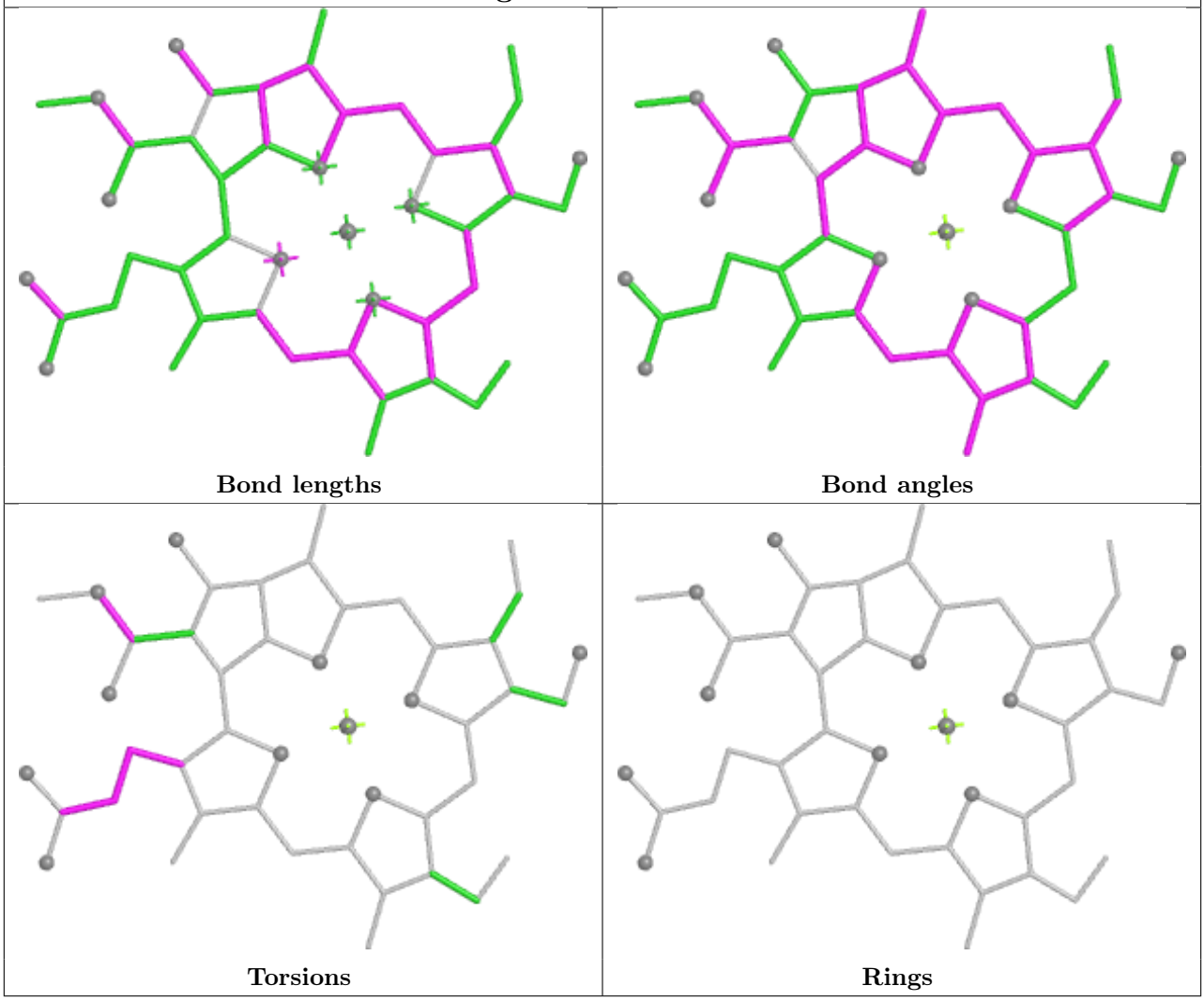
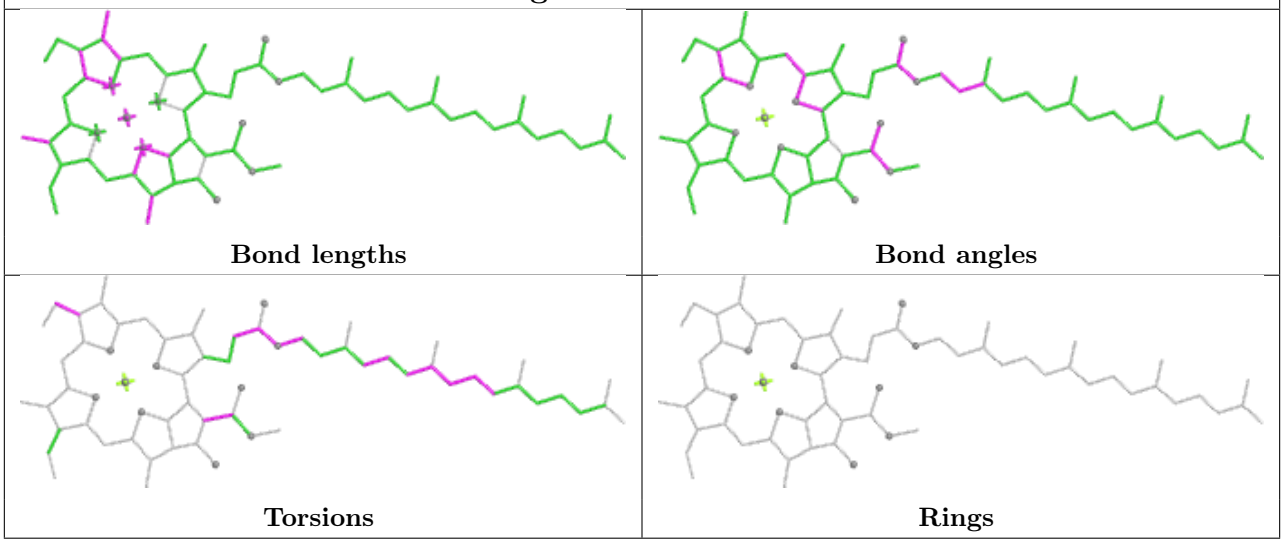


Rings

Ligand CHL 6 606



Ligand CLA c 513



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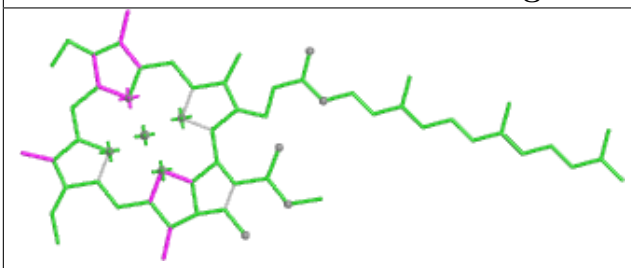
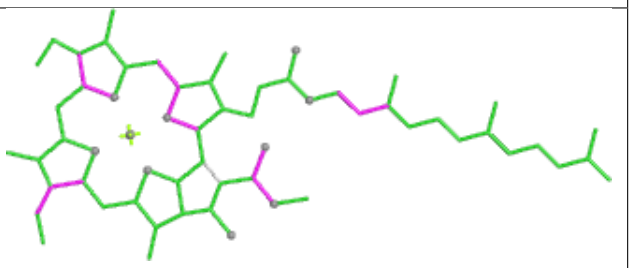
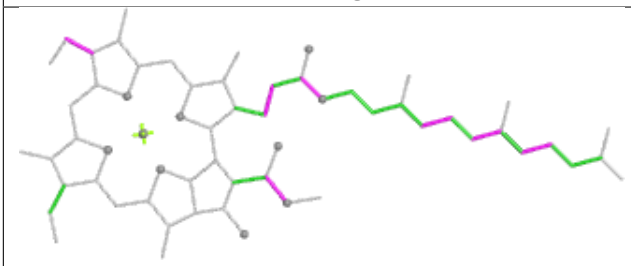
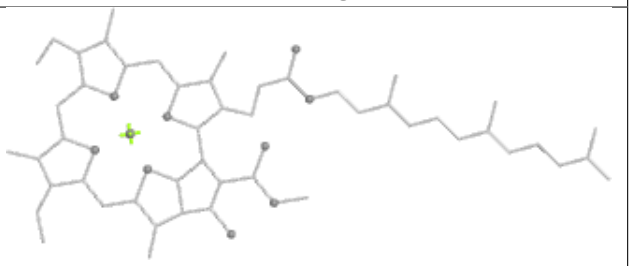
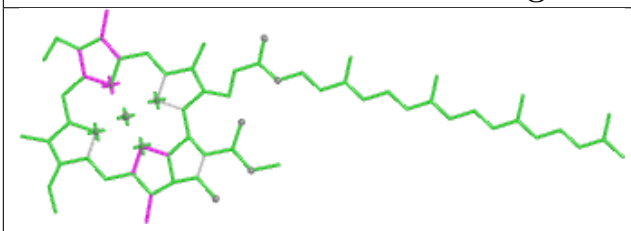
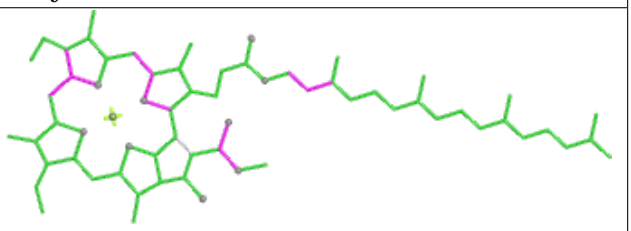
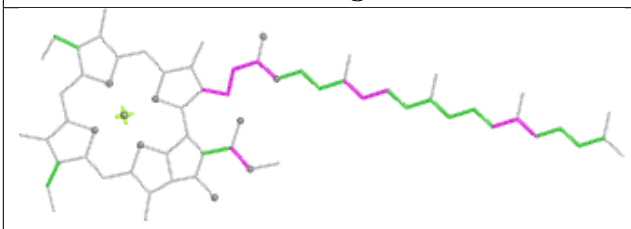
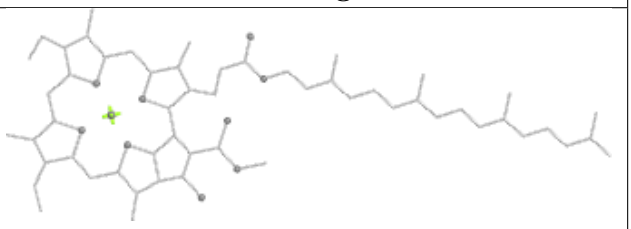
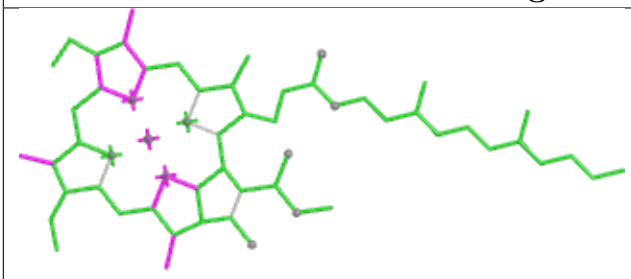
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 613



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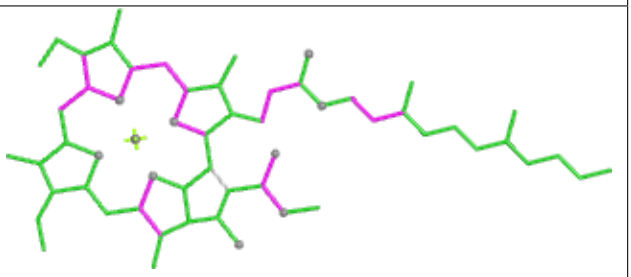

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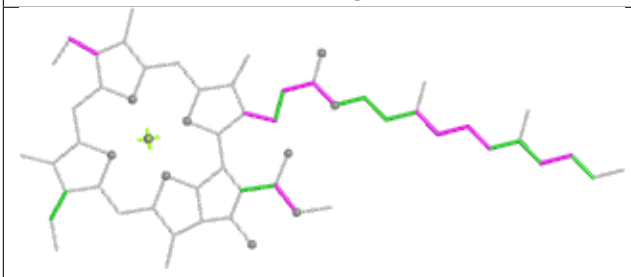

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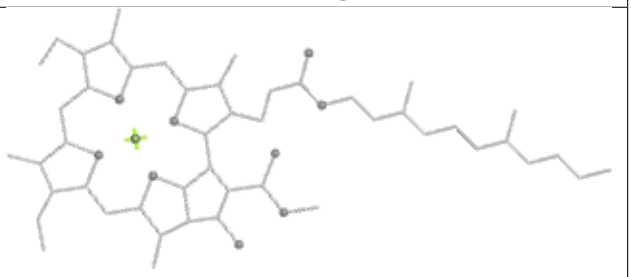
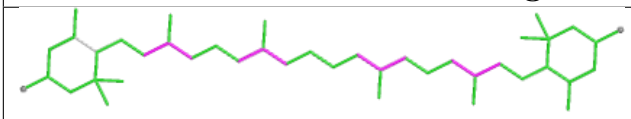


Rings

Ligand LUT Y 317



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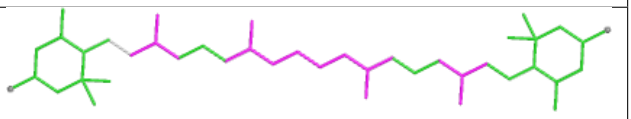

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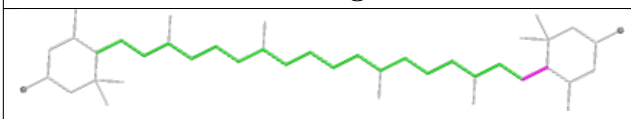

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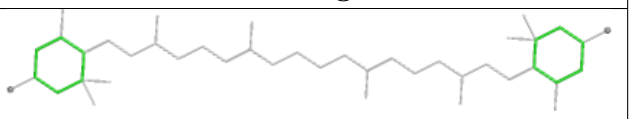
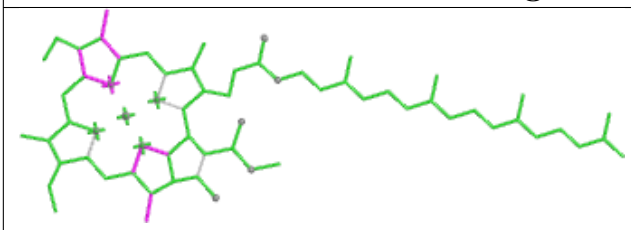


Rings

Ligand CLA C 504



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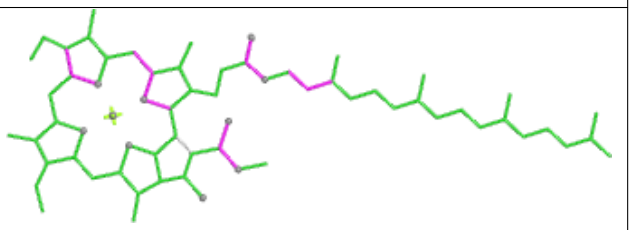

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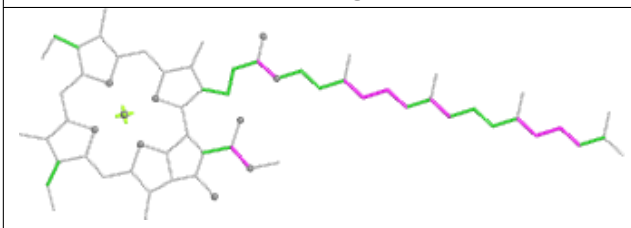

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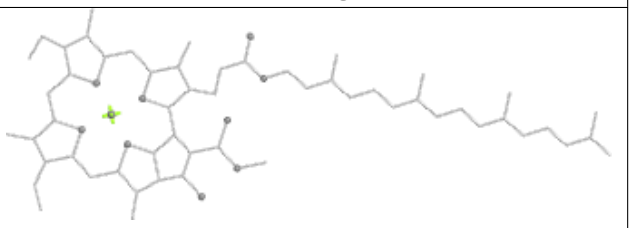
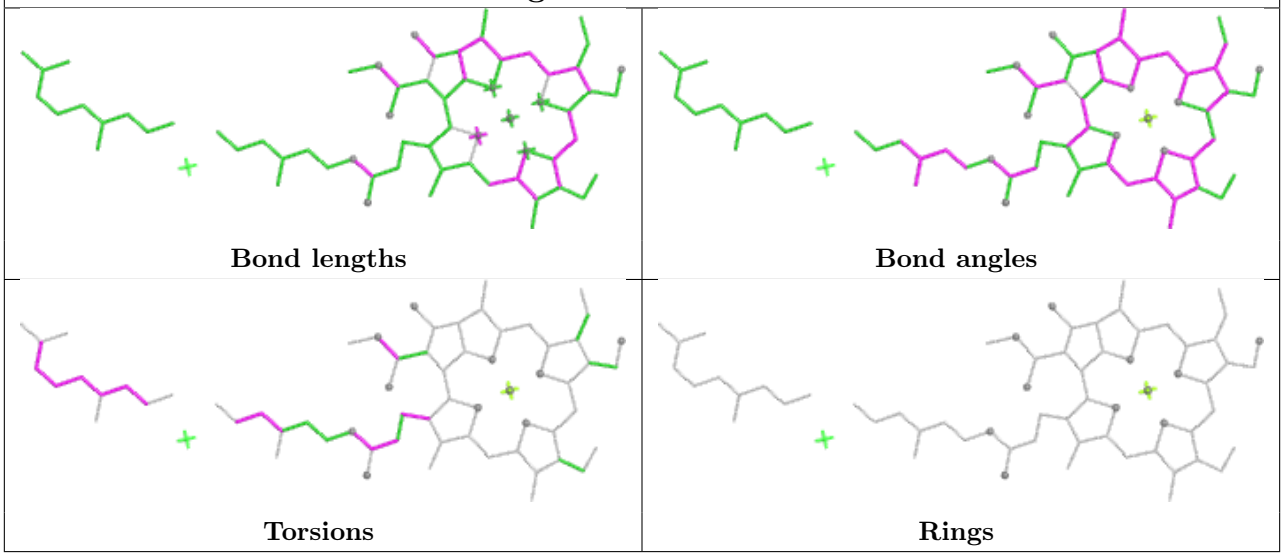
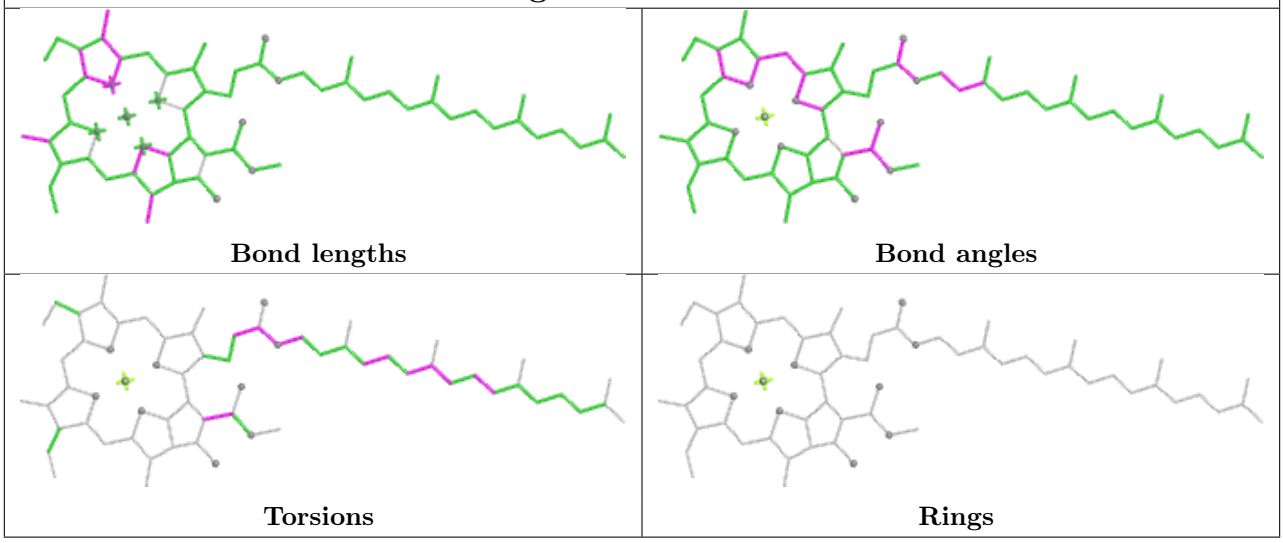


Rings

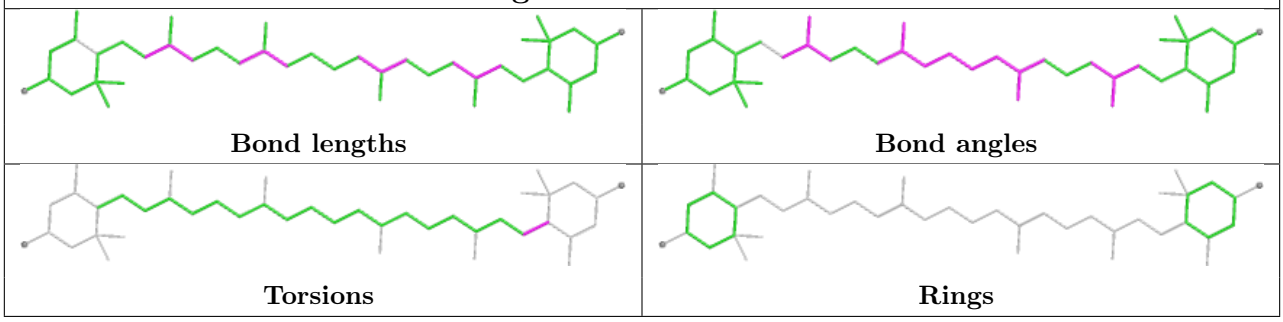
Ligand CHL n 601



Ligand CLA 1 512



Ligand LUT AB 311



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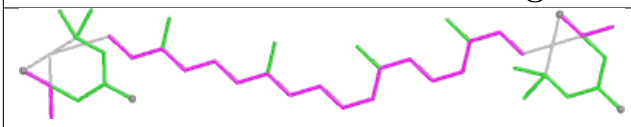
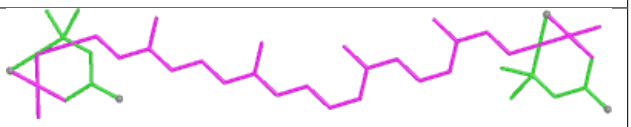
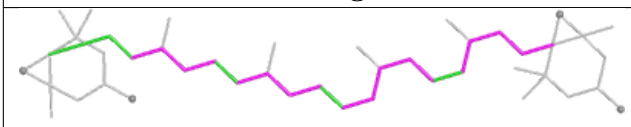
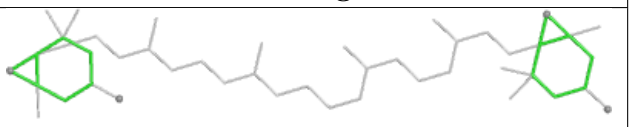
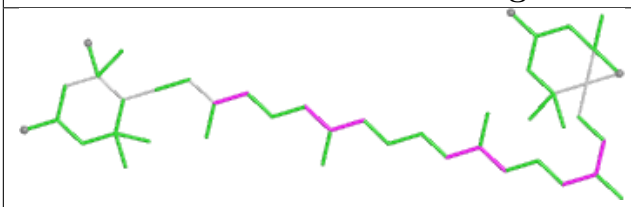
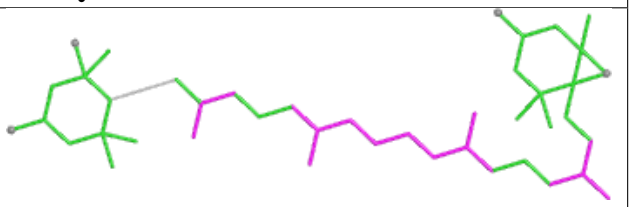
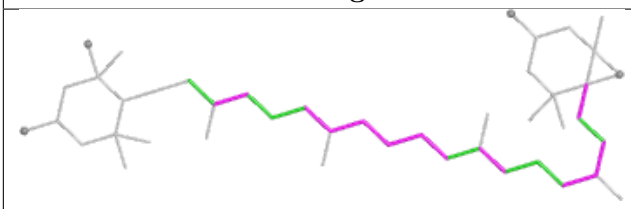
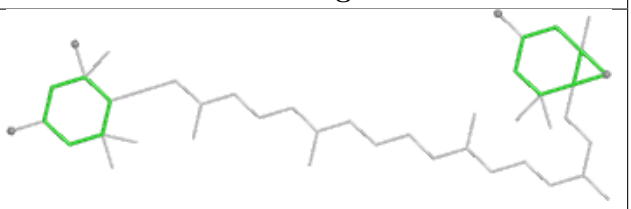
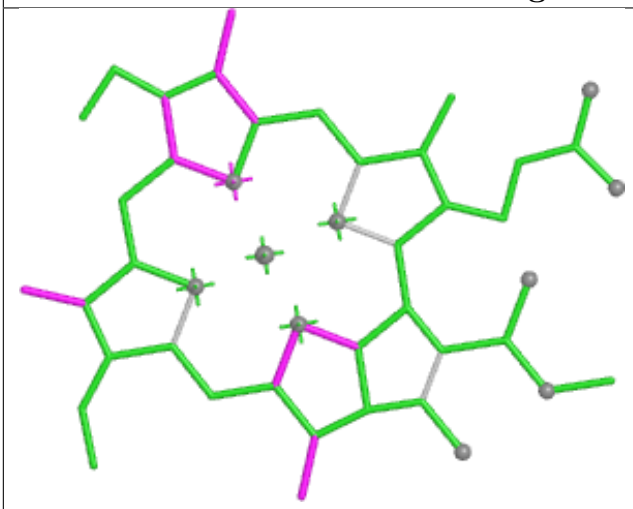
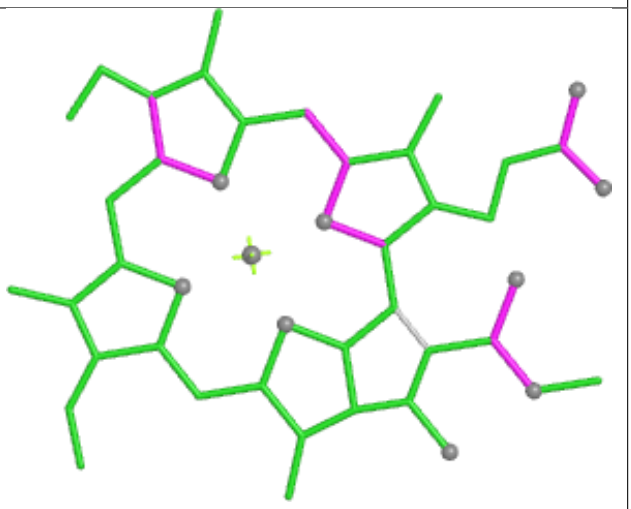
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX BQ 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

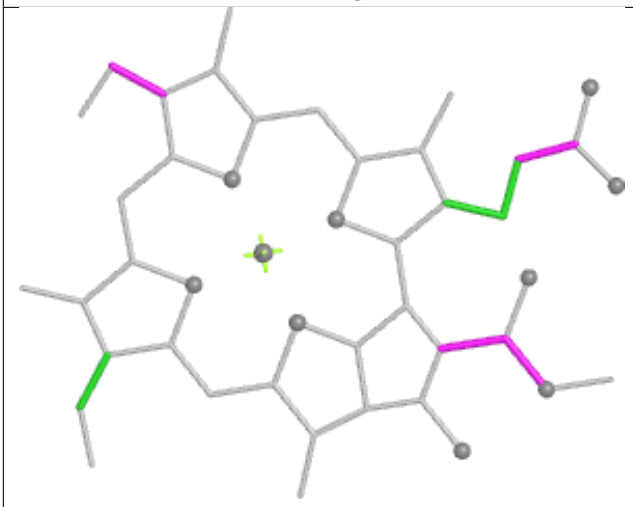
Ligand CLA 0 612



Bond lengths



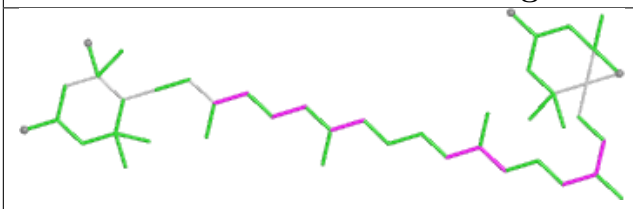
Bond angles



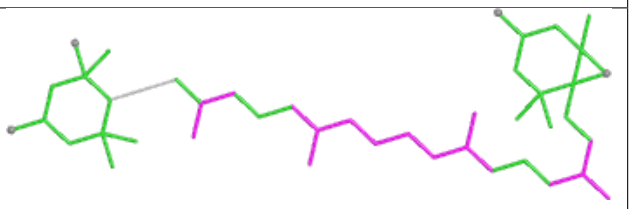
Torsions

Rings

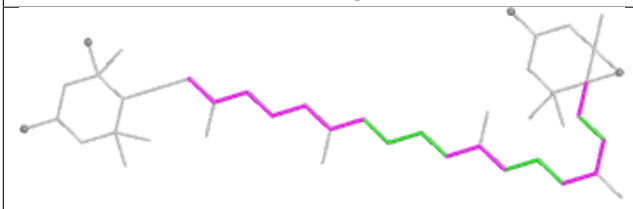
Ligand NEX G 617



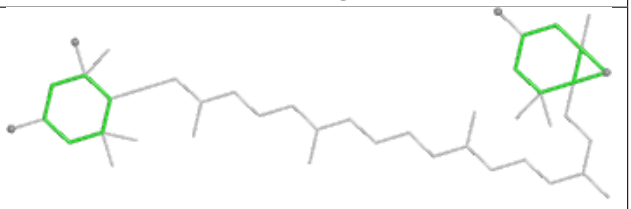
Bond lengths



Bond angles

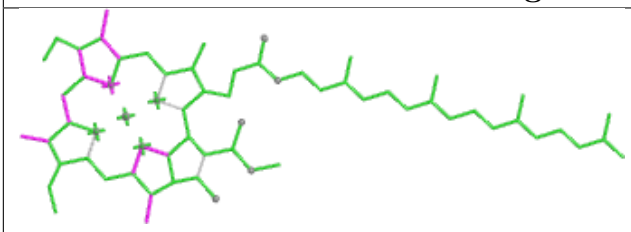


Torsions



Rings

Ligand CLA B 606



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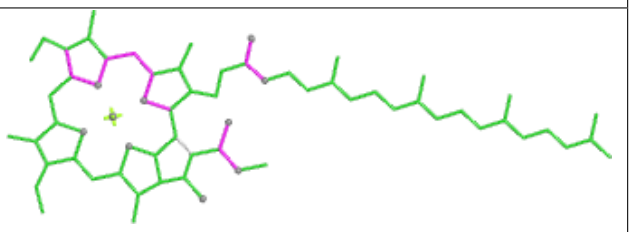
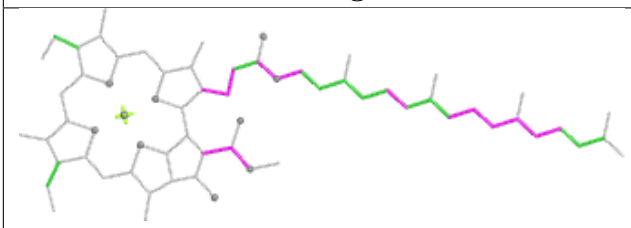


Bond angles



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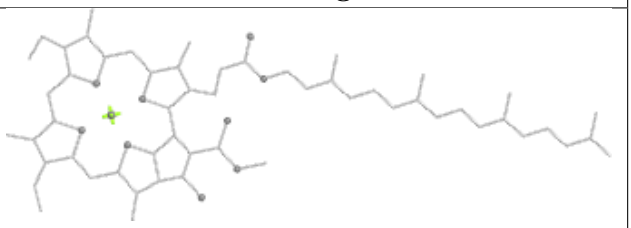


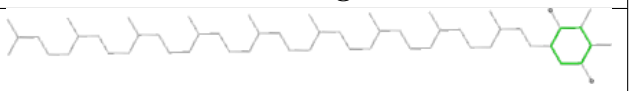
Rings

Ligand PL9 2 404

Bond lengths

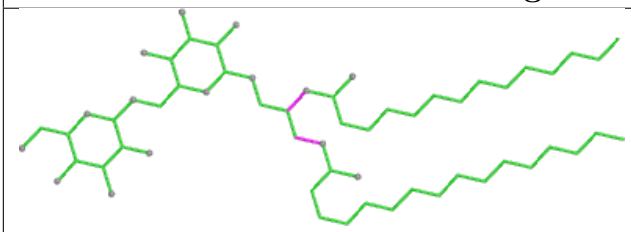
Bond angles

Torsions



Rings

Ligand DGD 1 518



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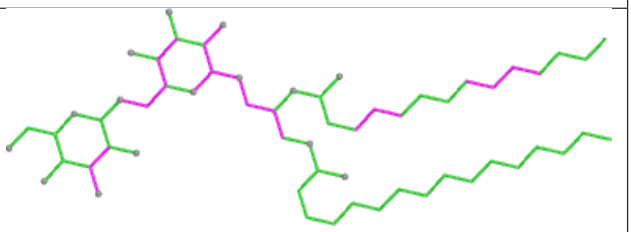
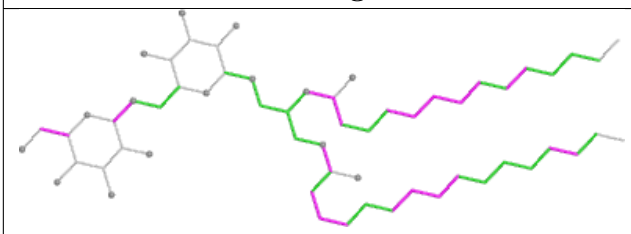


Bond angles



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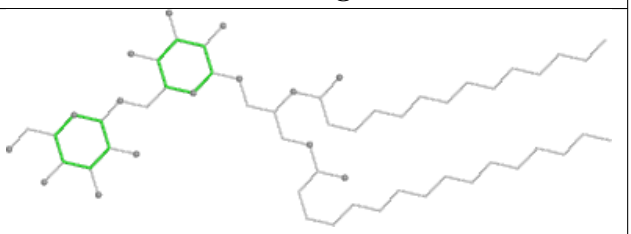
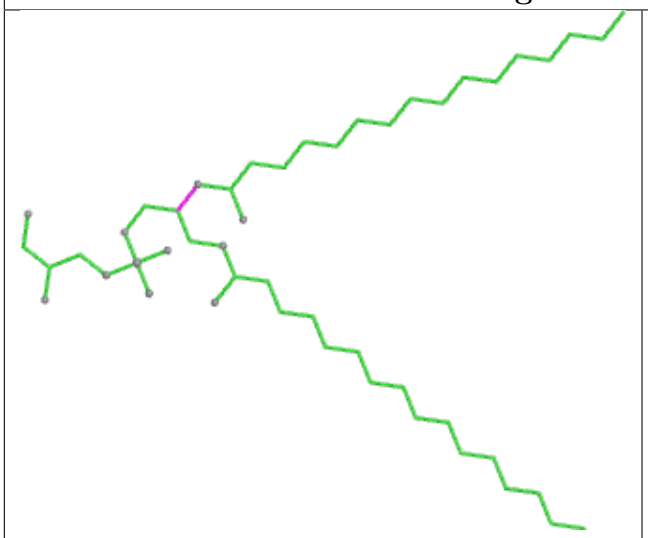


Rings

Ligand LHG Ba 319



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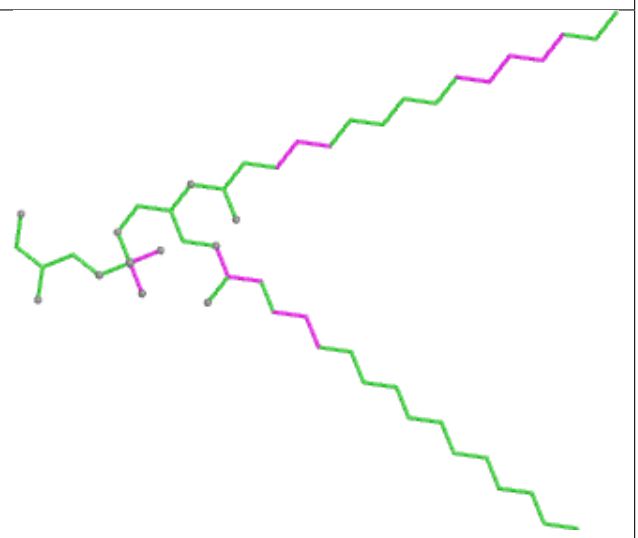
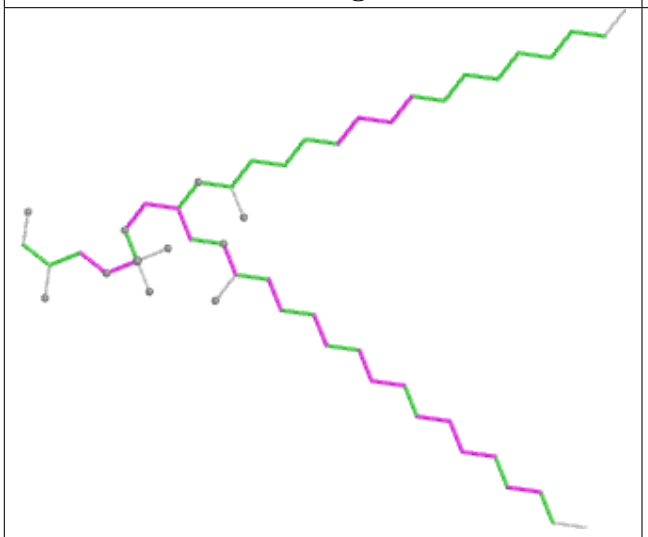


Bond angles



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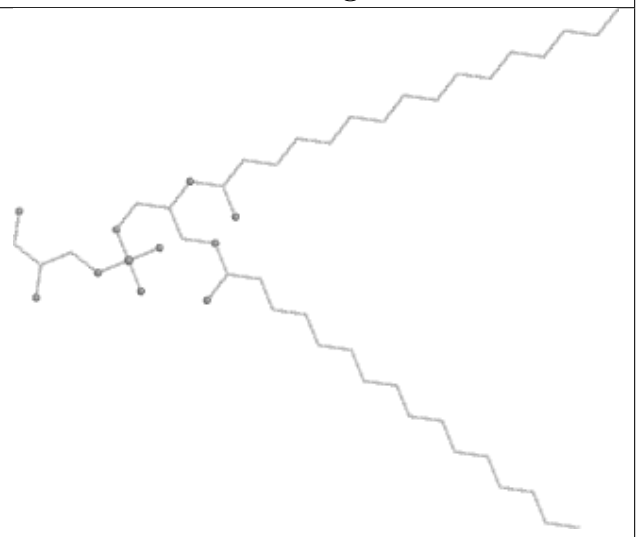
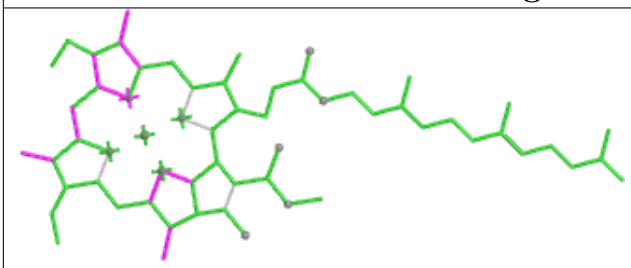
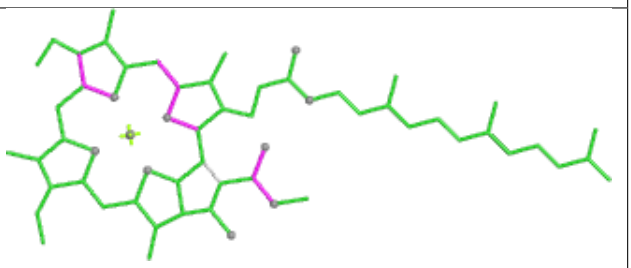
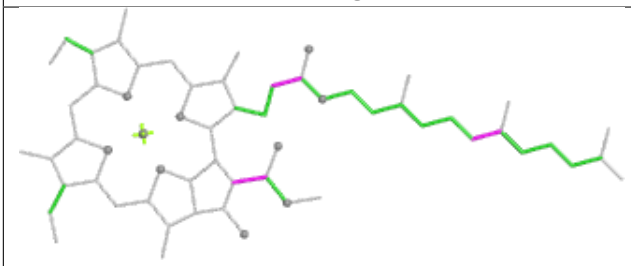
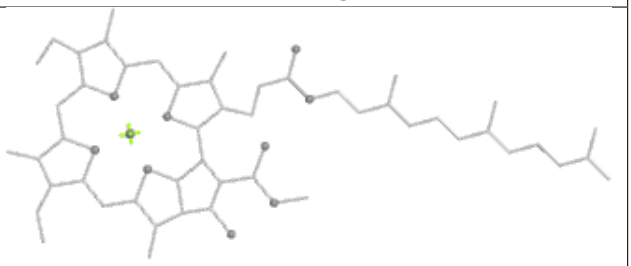
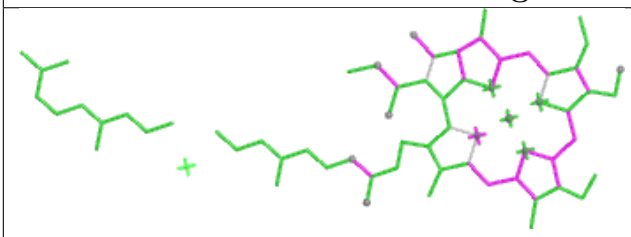
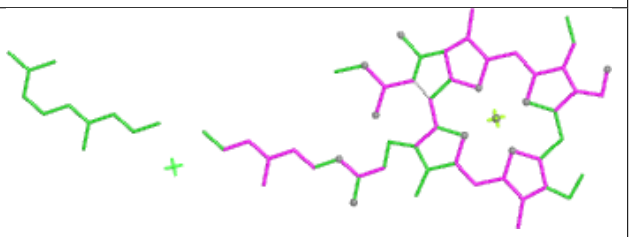
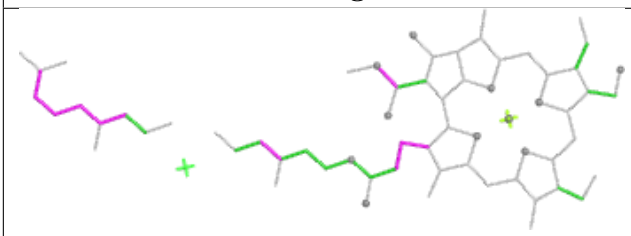
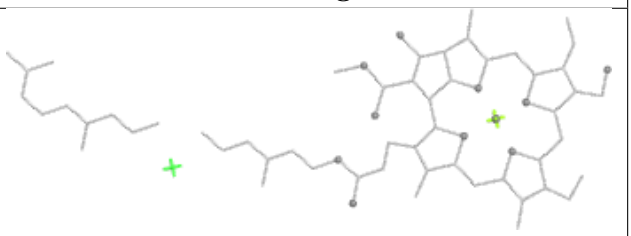
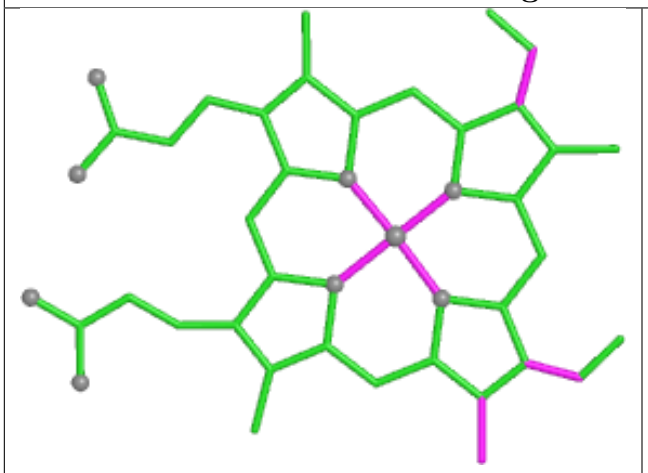


Rings

Ligand CLA N 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL BB 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM F 102



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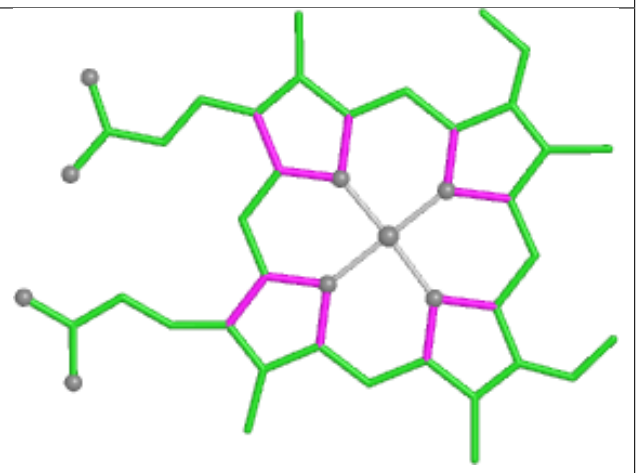

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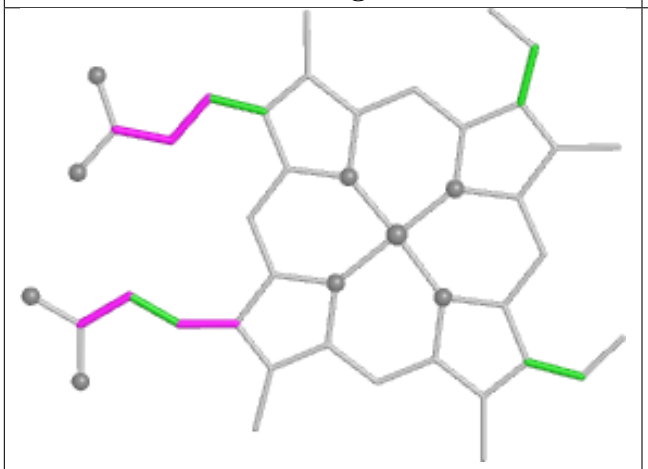

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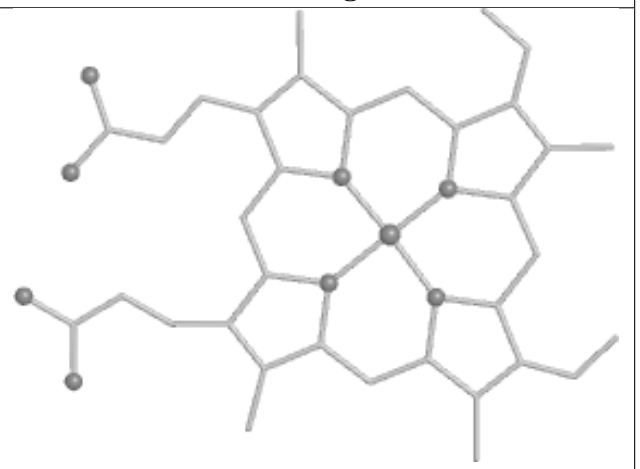
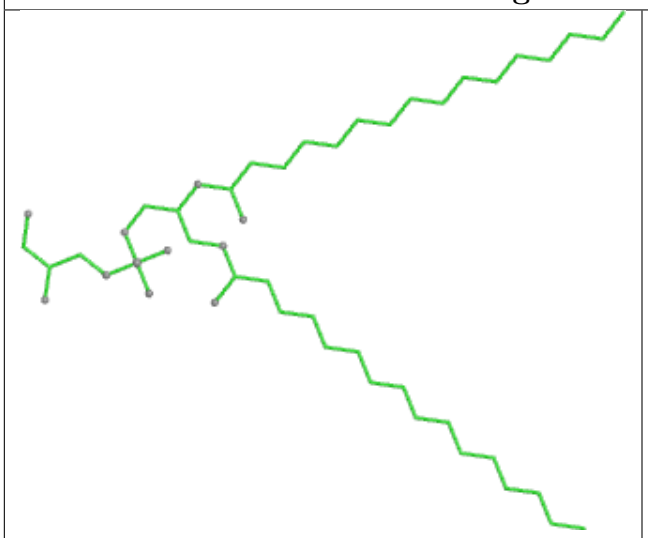


Rings

Ligand LHG BF 520



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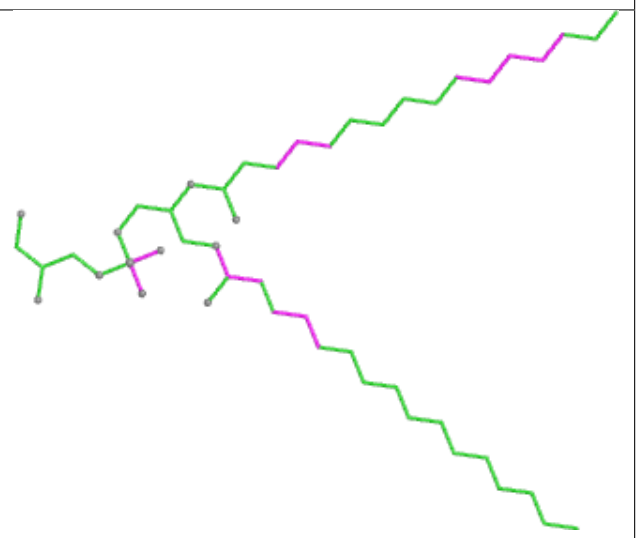
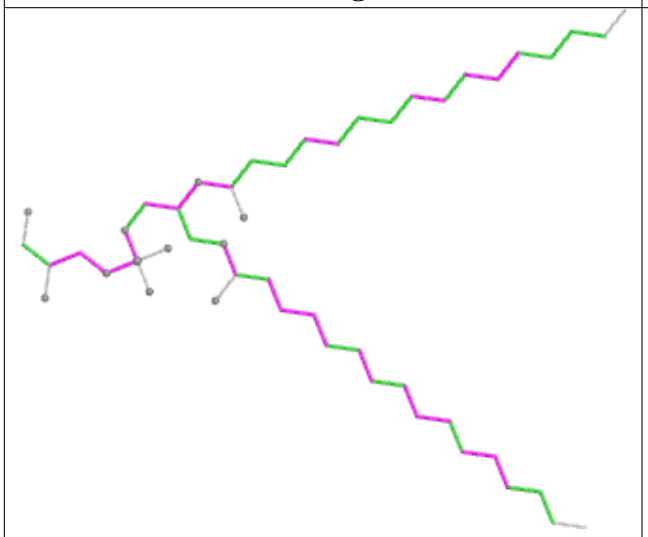


Bond angles



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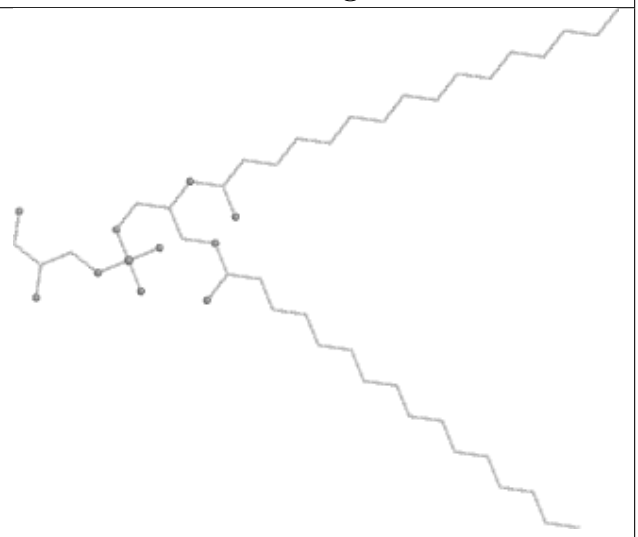
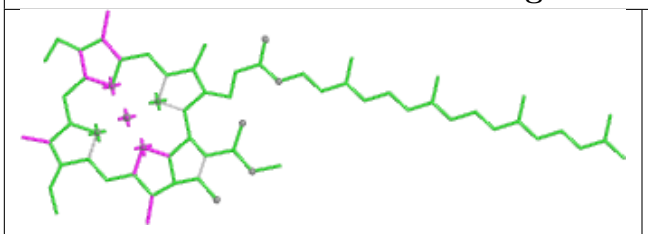


Rings

Ligand CLA B 612



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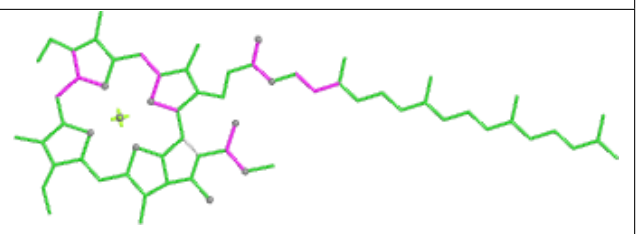
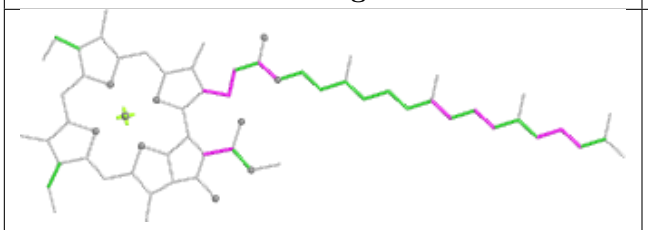


Bond angles



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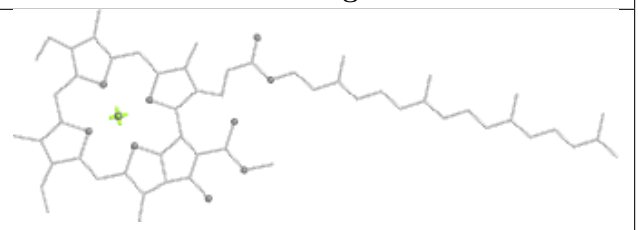
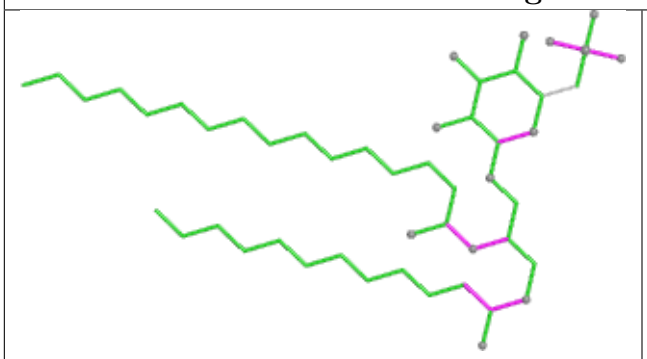


Rings

Ligand SQD D 406



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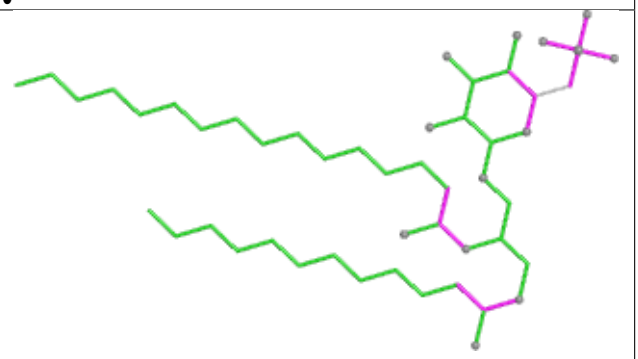
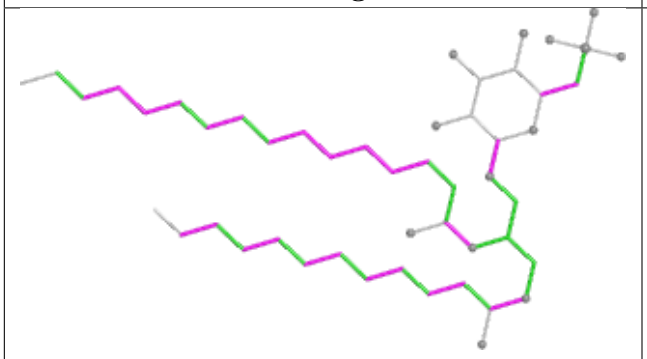
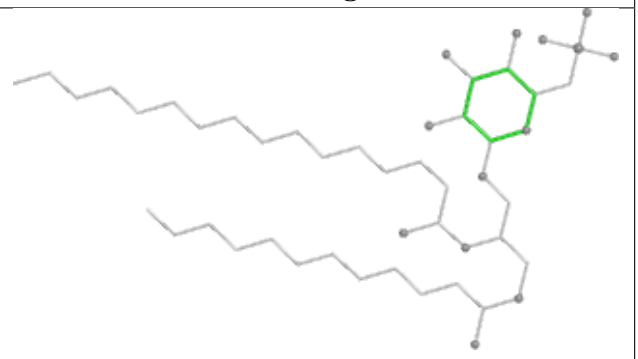


Bond angles

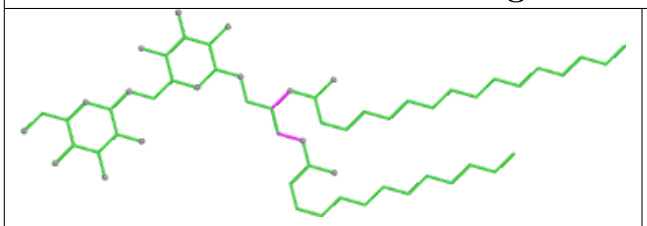


Torsions



Rings

Ligand DGD BD 401



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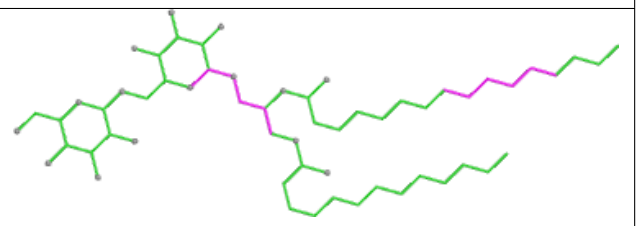
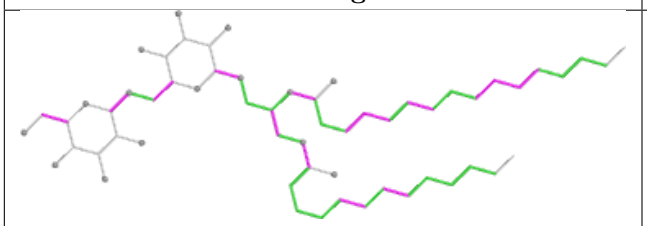


Bond angles



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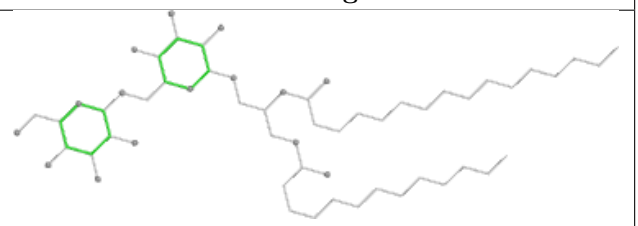
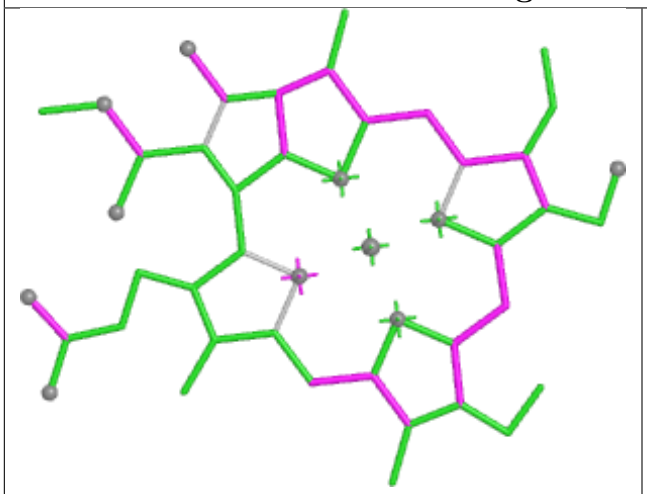


Rings

Ligand CHL BJ 605



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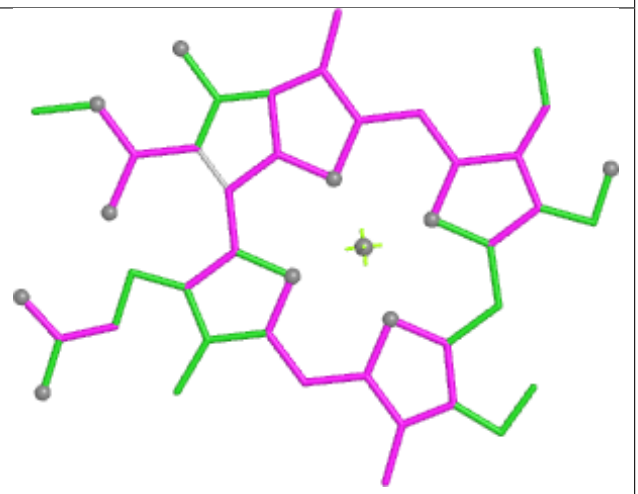
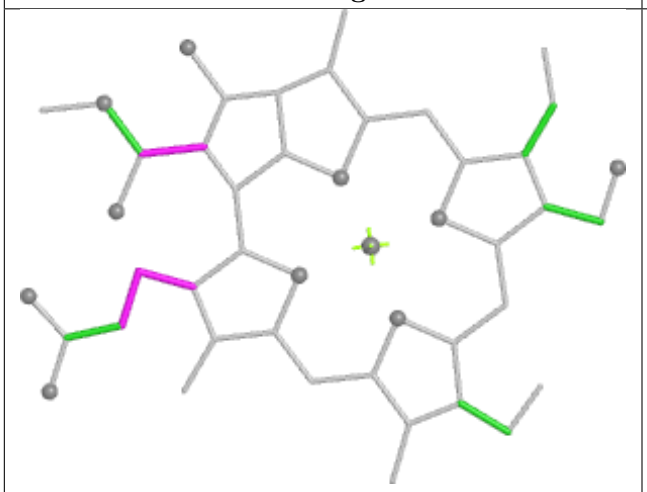


Bond angles



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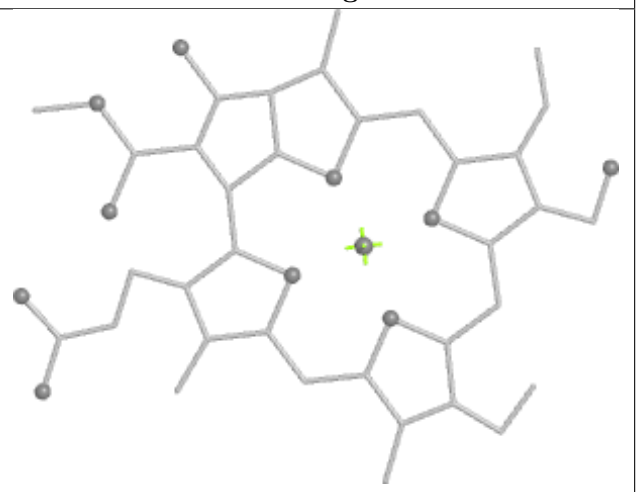
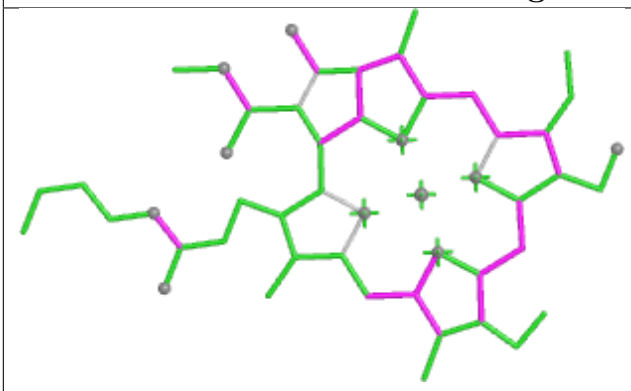


Rings

Ligand CHL g 606



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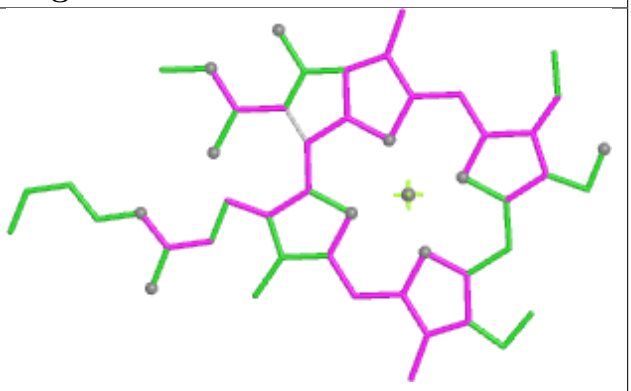
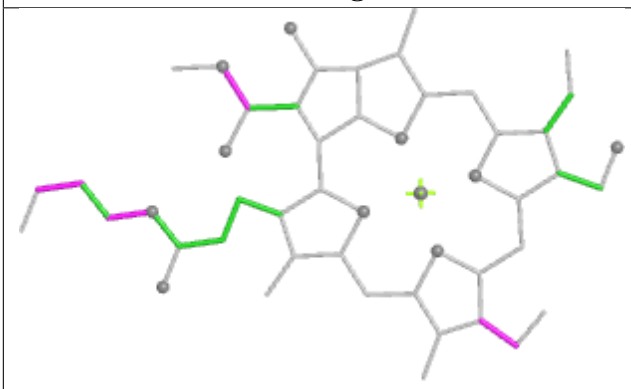


Bond angles



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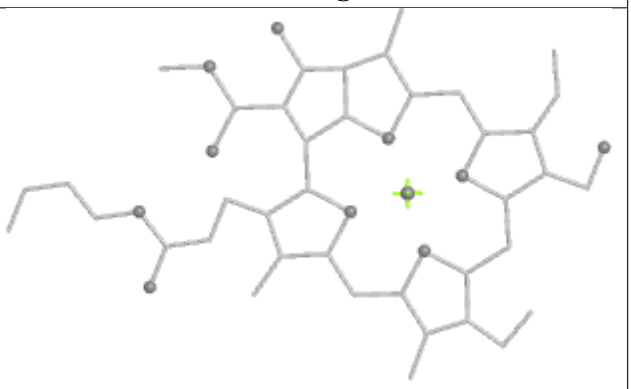
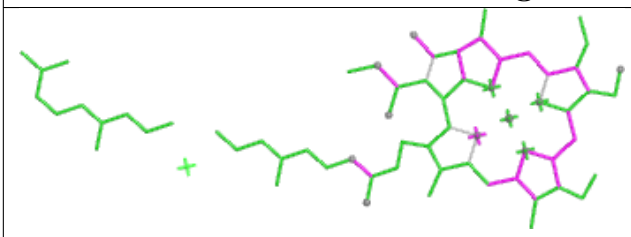


Rings

Ligand CHL Ba 309



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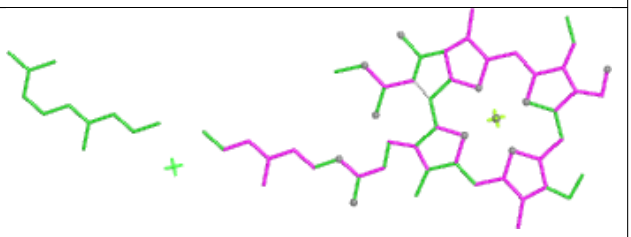
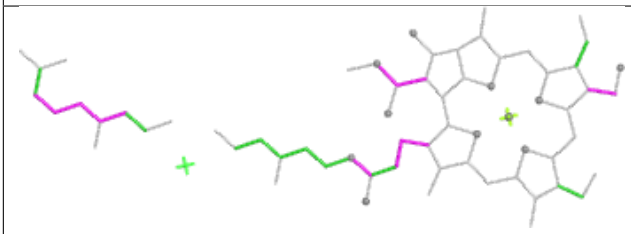


Bond angles



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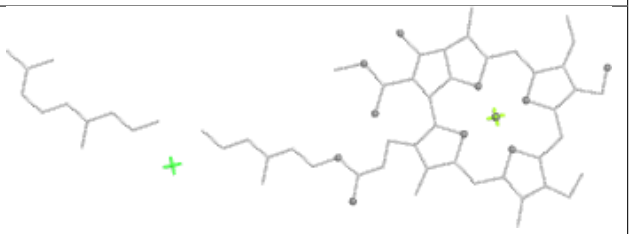
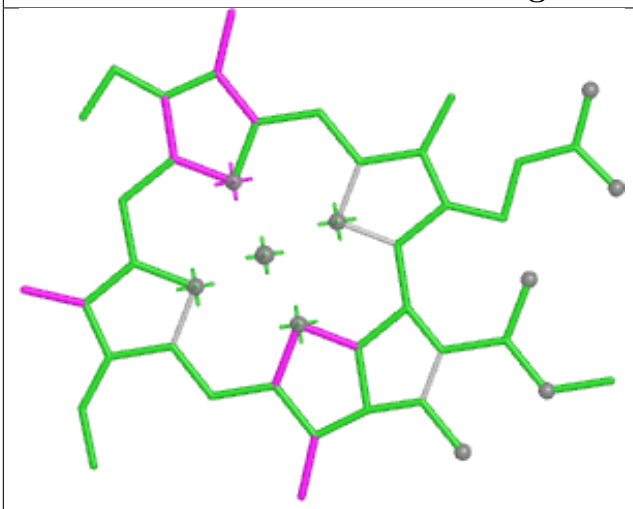
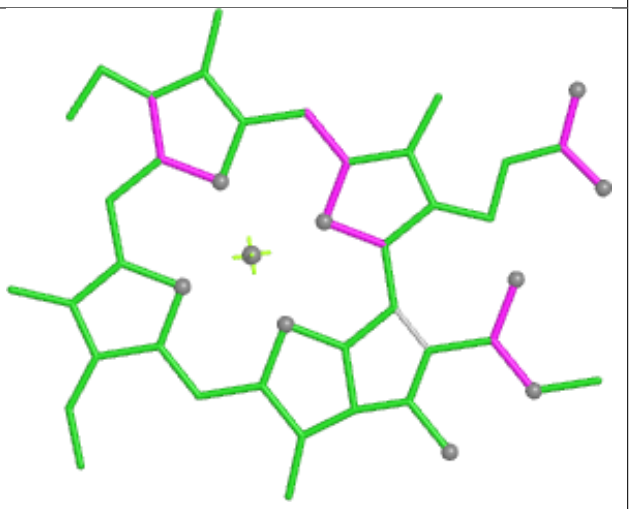


Rings

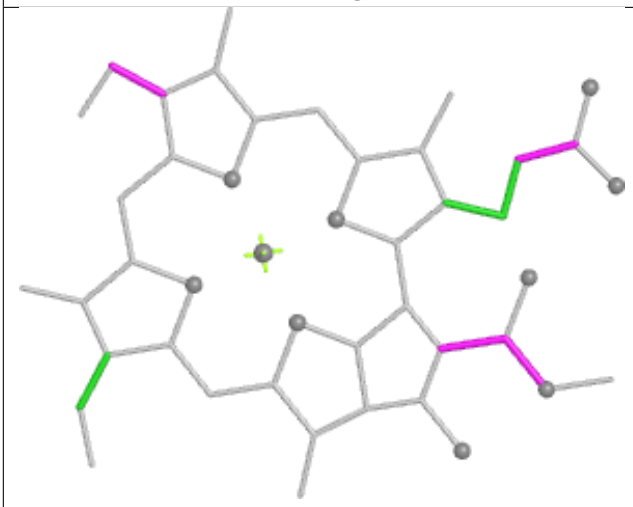
Ligand CLA 6 612



Bond lengths

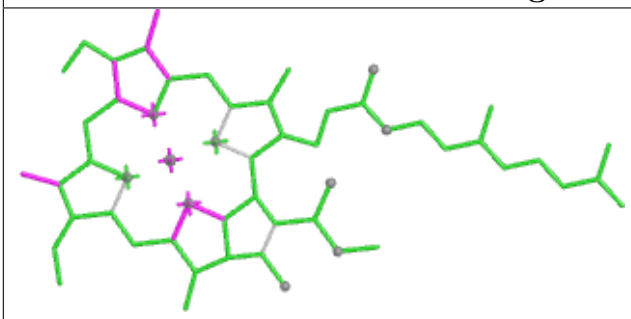
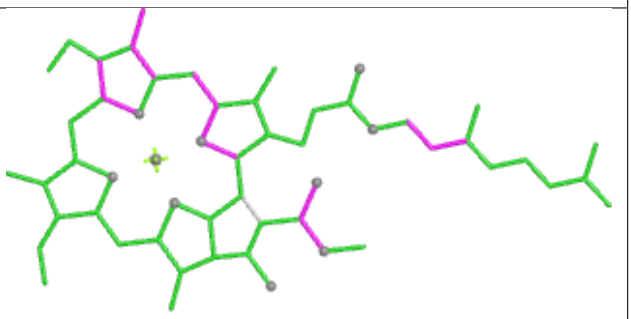
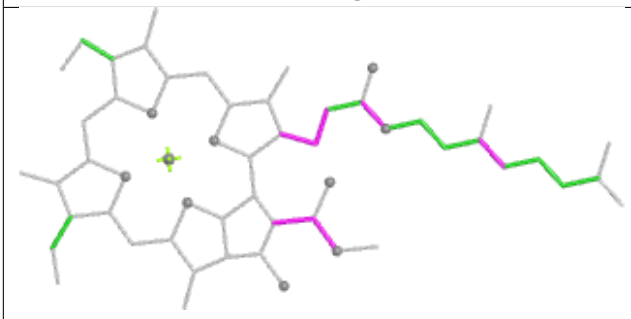
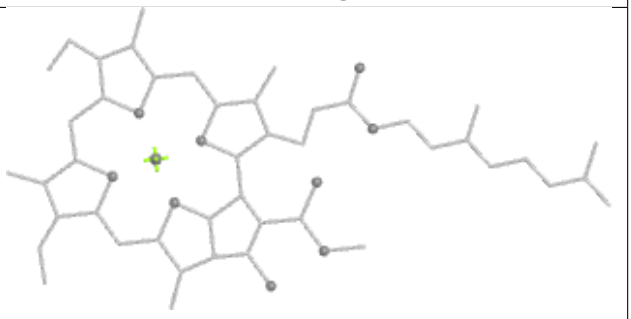


Bond angles



Torsions

Rings

Ligand CLA 9 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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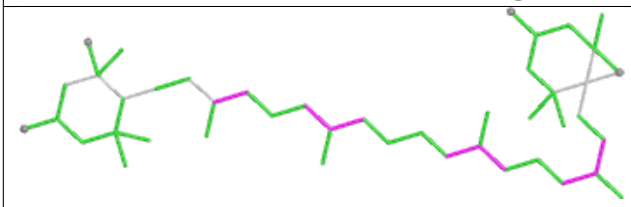
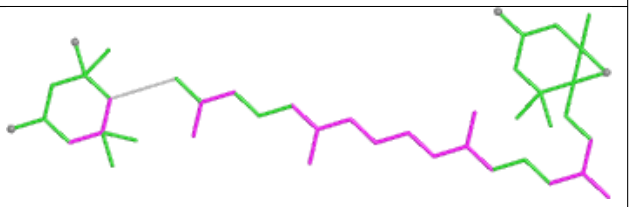
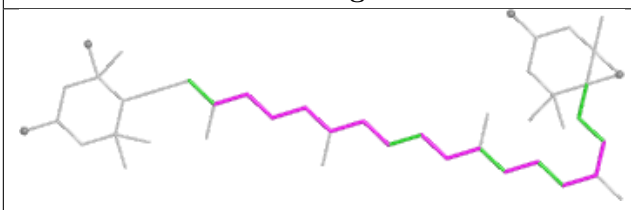
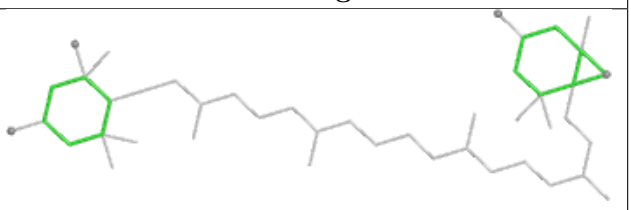
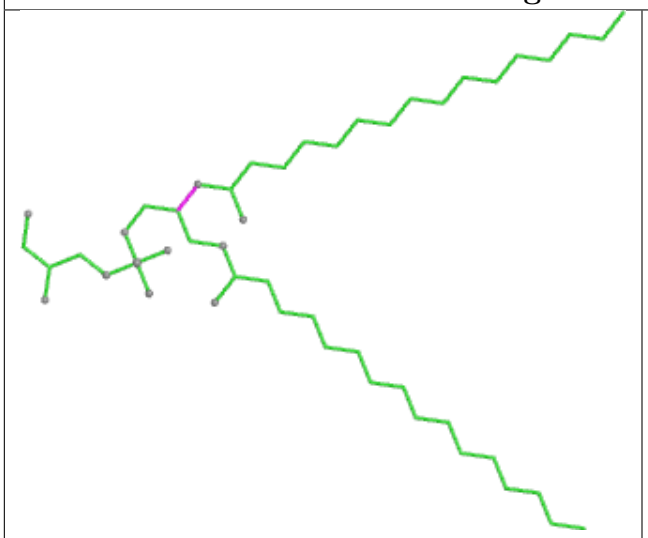
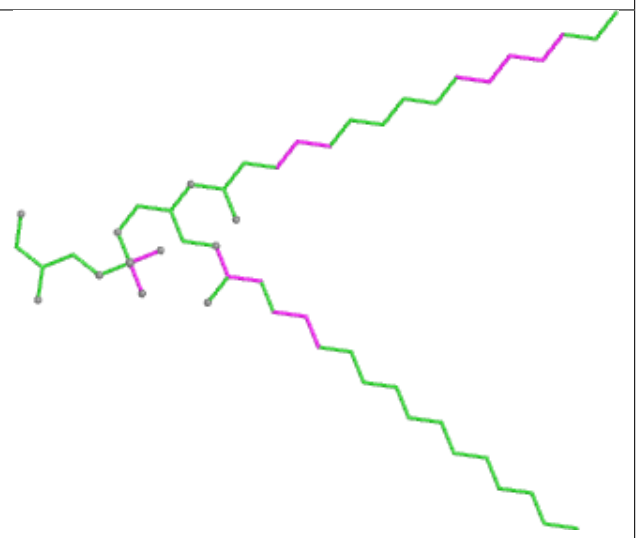
 Bond lengths	 Bond angles
 Torsions	 Rings

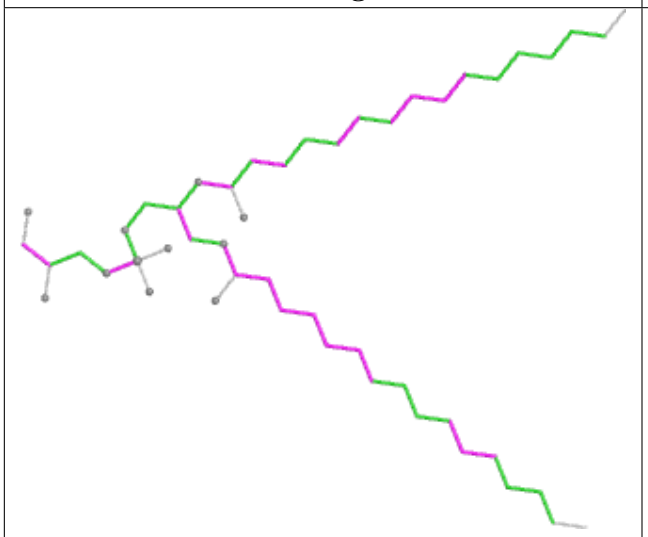
Ligand LHG C 521



Bond lengths



Bond angles



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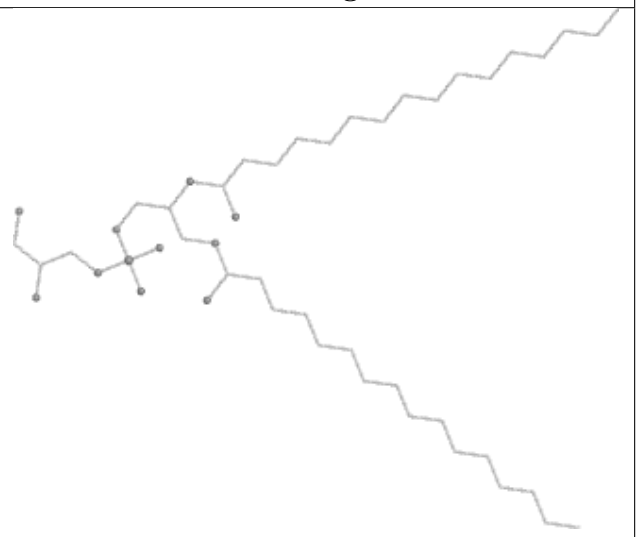
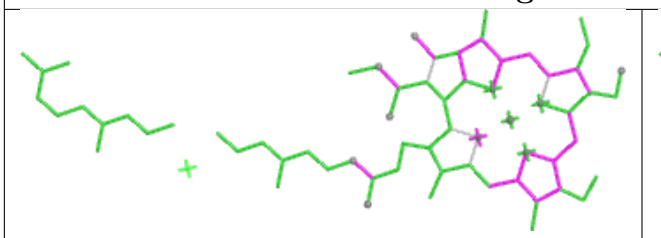


Rings

Ligand CHL Ba 310



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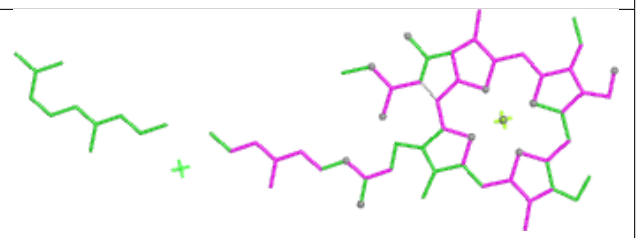
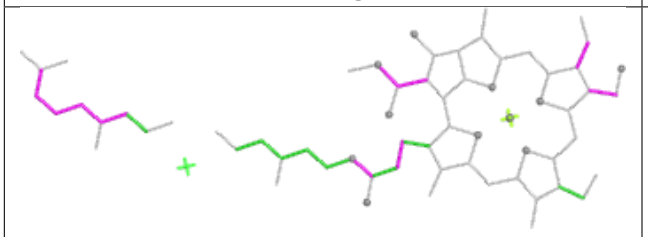


Bond angles



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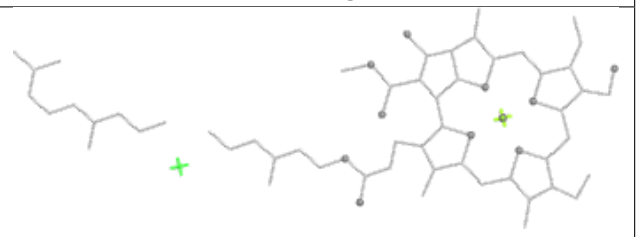
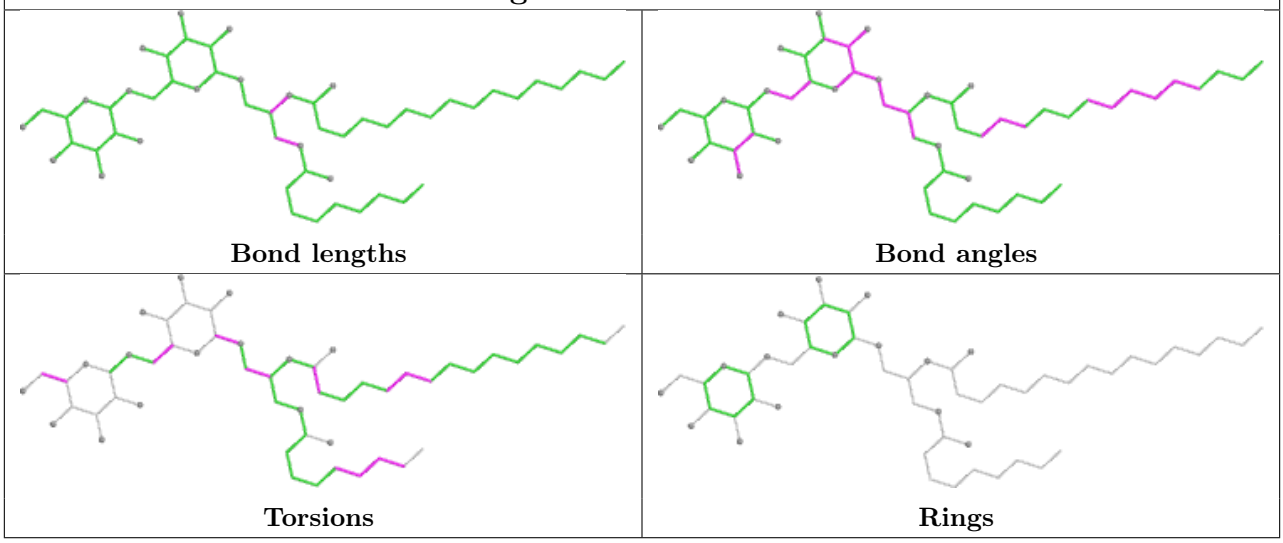
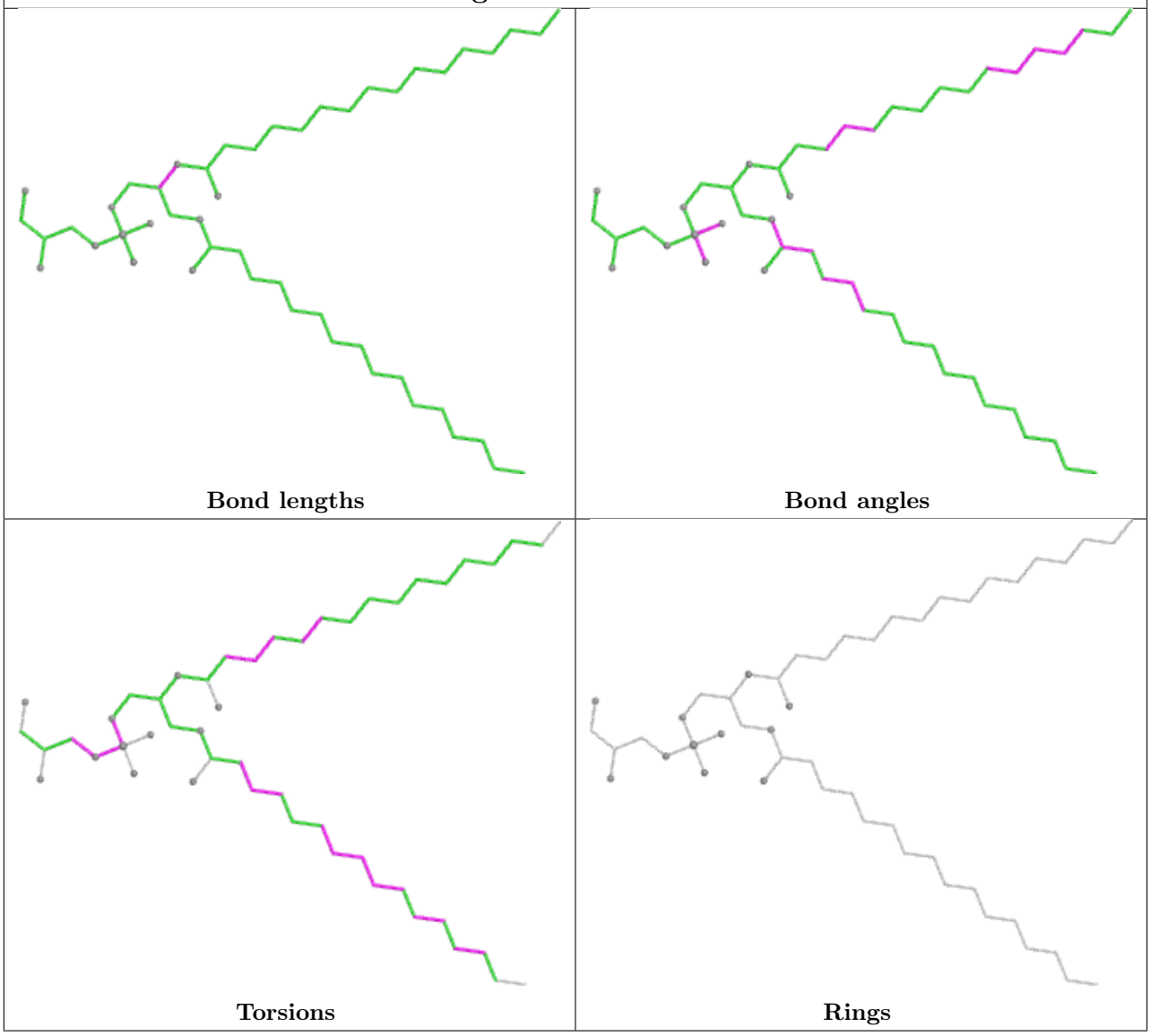


Rings

Ligand DGD BF 517



Ligand LHG d 404



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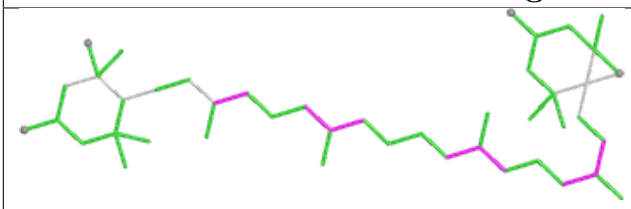
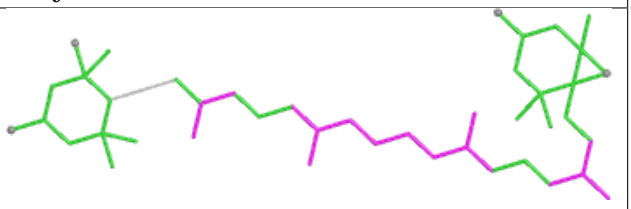
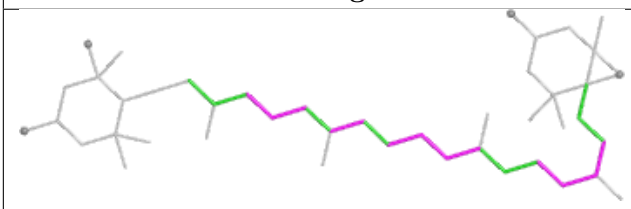
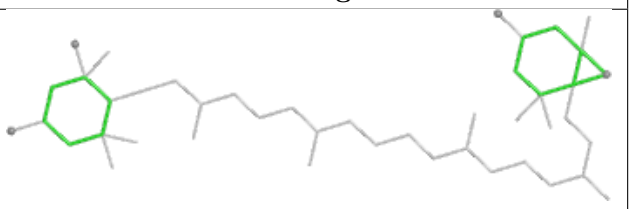
 Bond lengths	 Bond angles
 Torsions	 Rings

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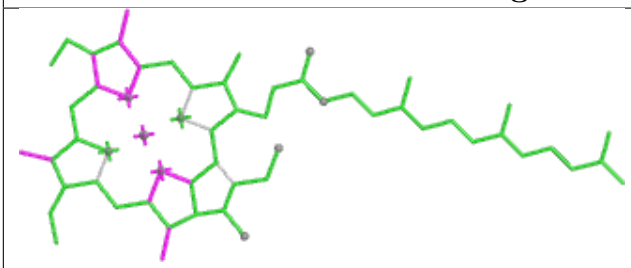
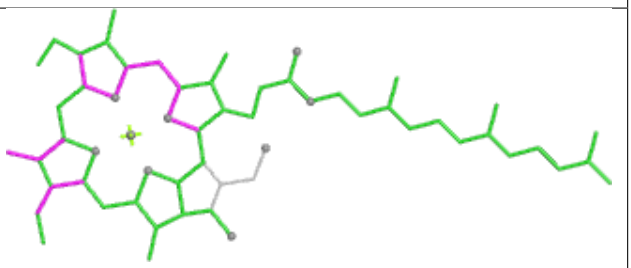
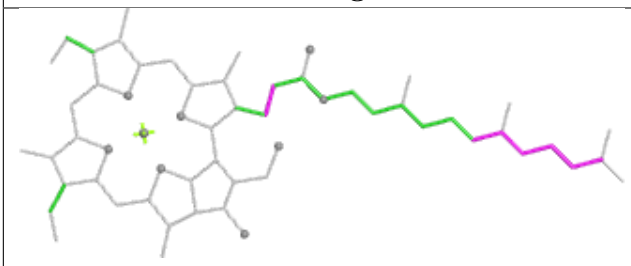
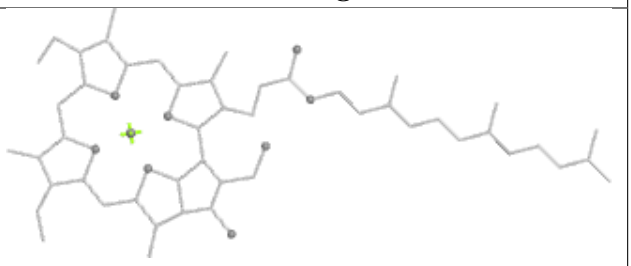
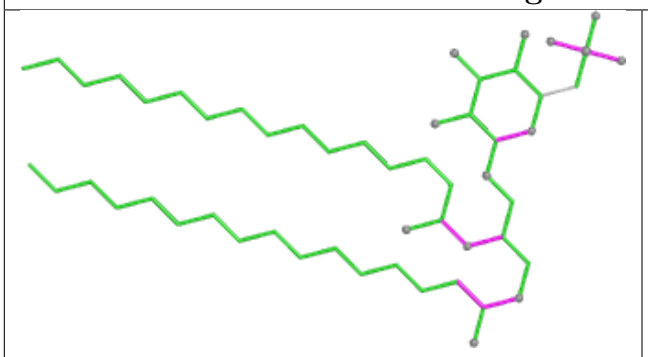
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD R 411



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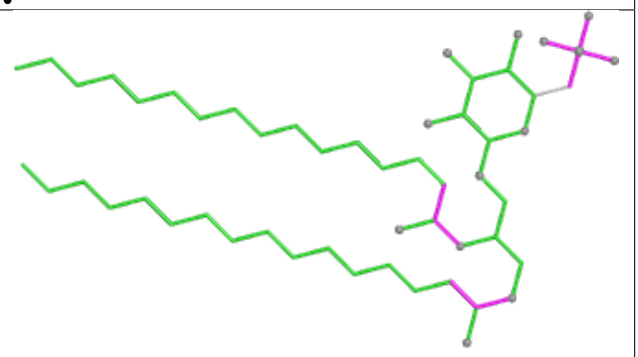
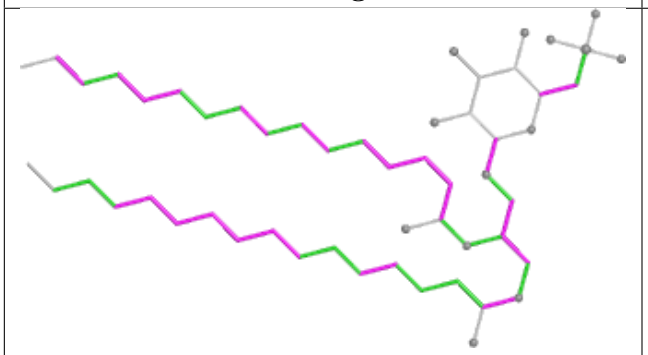


Bond angles



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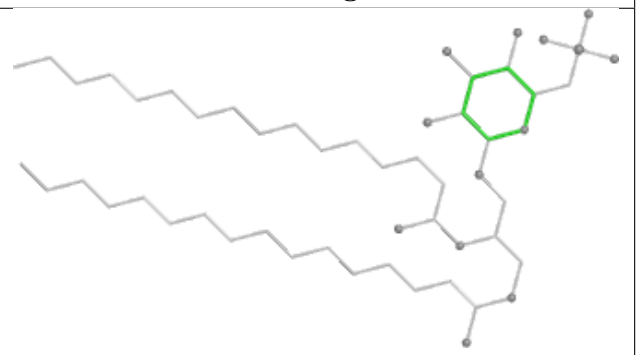
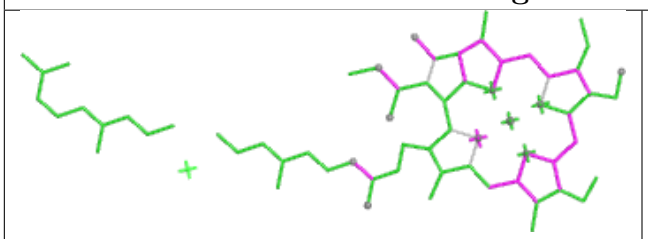
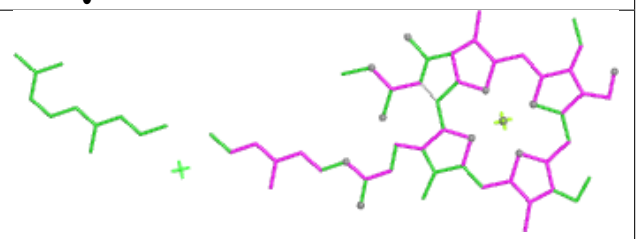


Rings

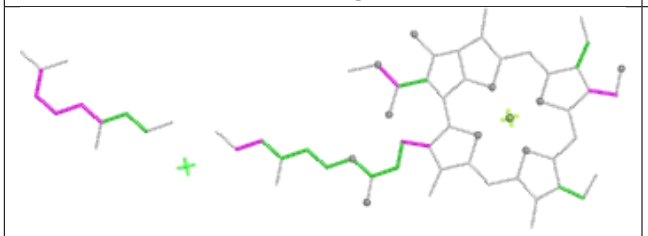
Ligand CHL BQ 608



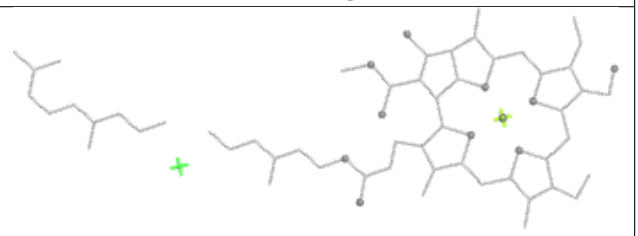
Bond lengths



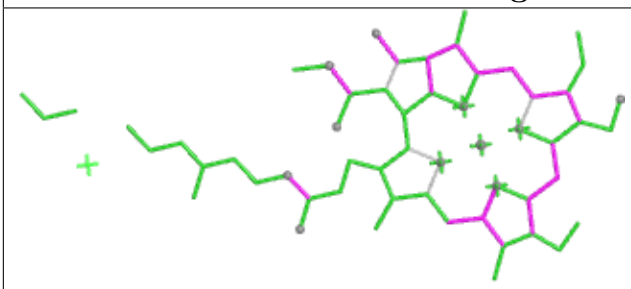
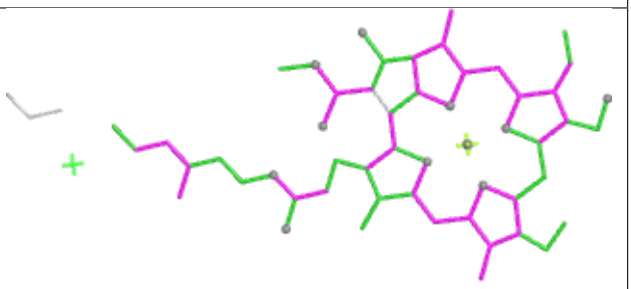
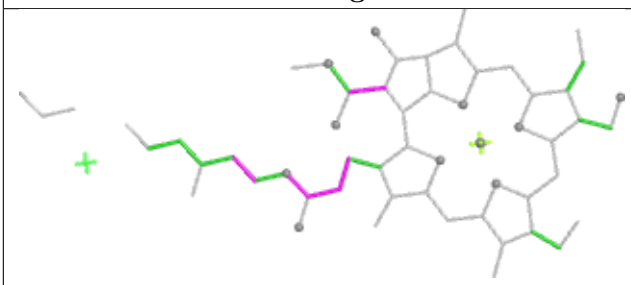
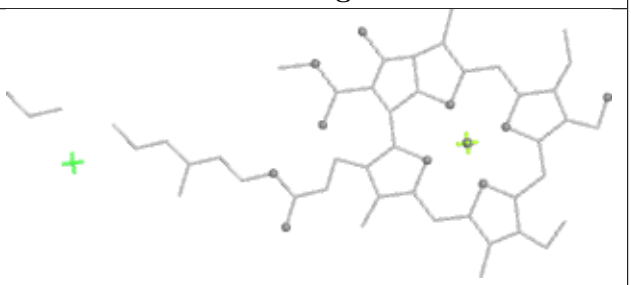
Bond angles

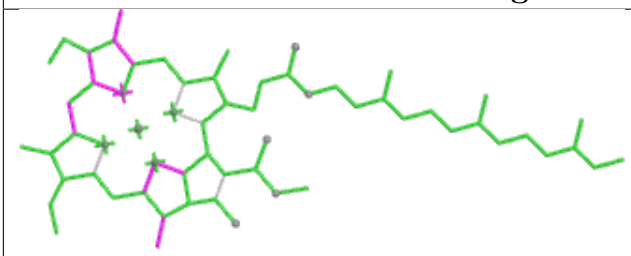
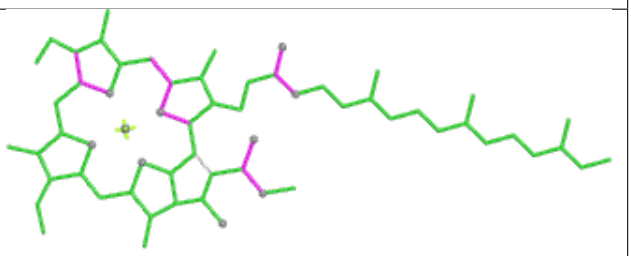
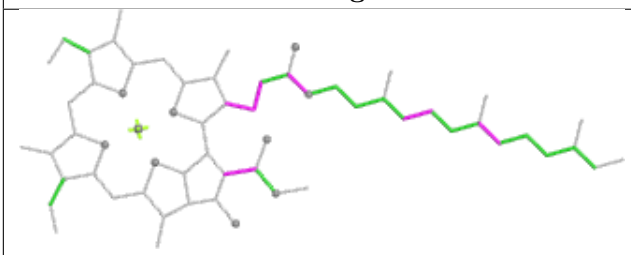
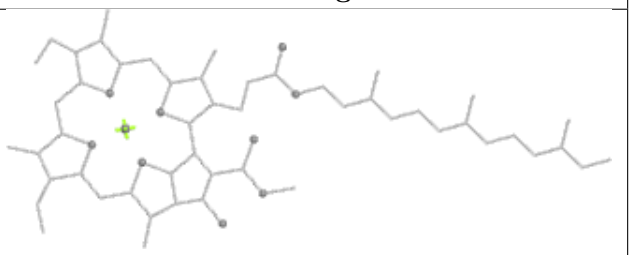


Torsions

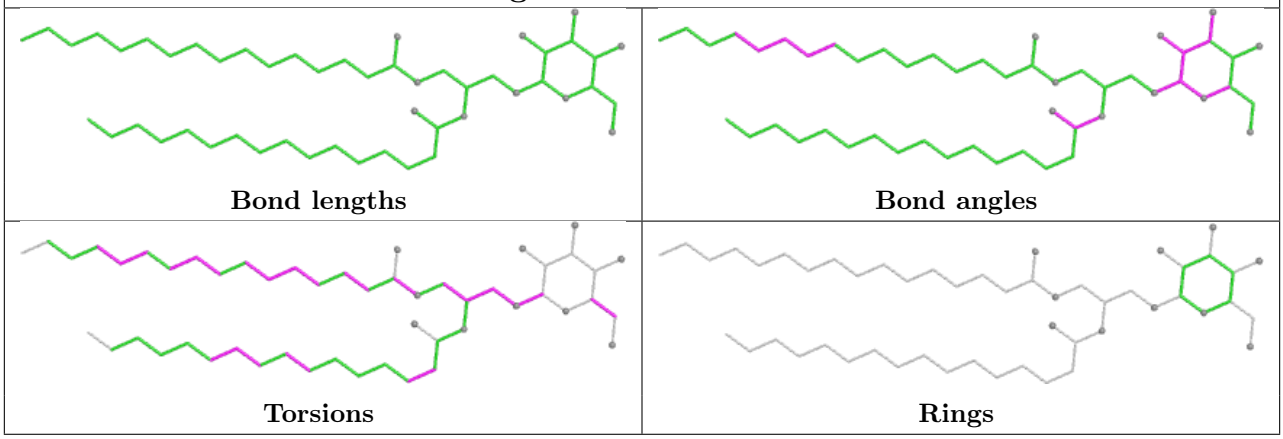


Rings

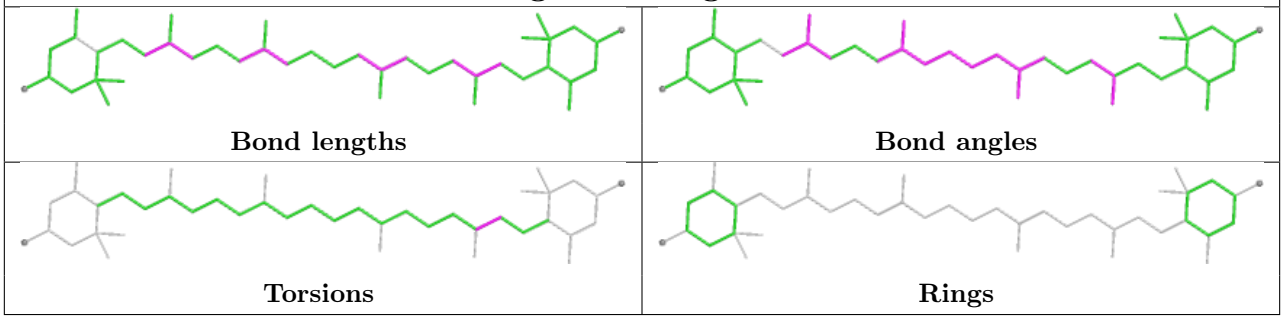
Ligand CHL BV 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BV 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

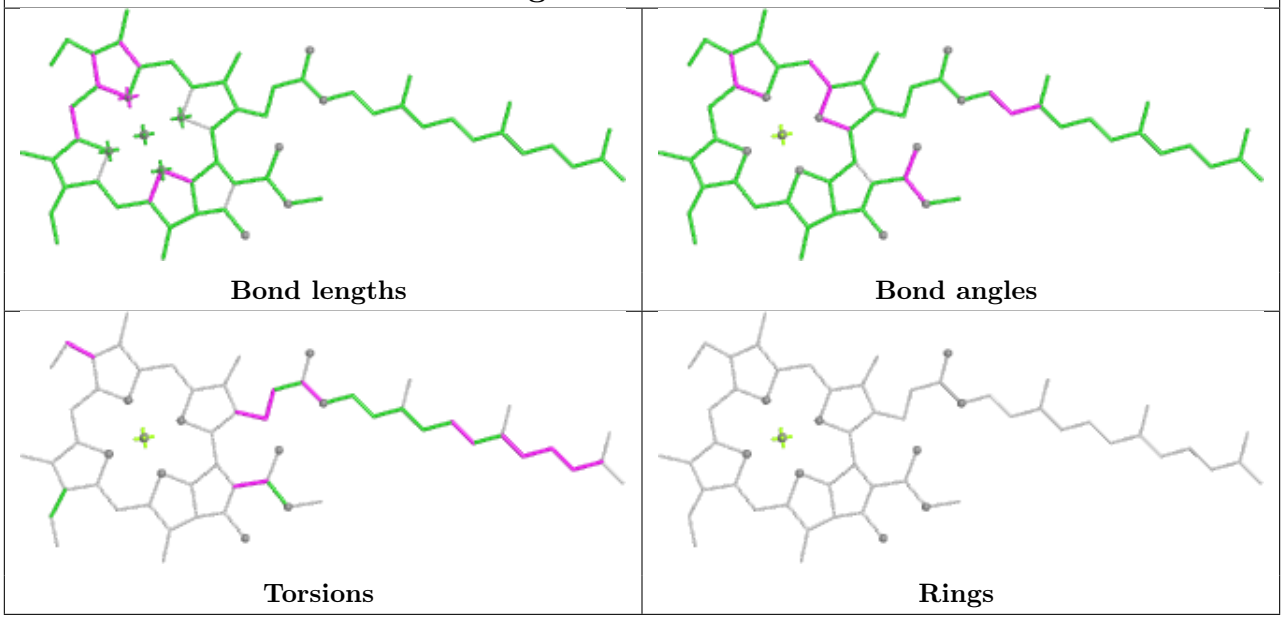
Ligand LMG BF 501



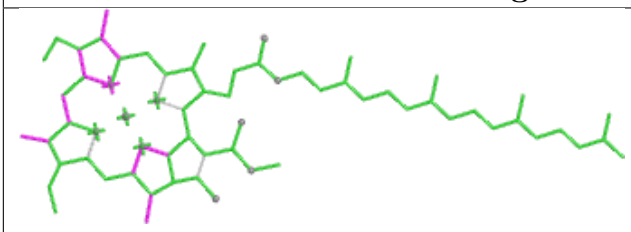
Ligand LUT g 615



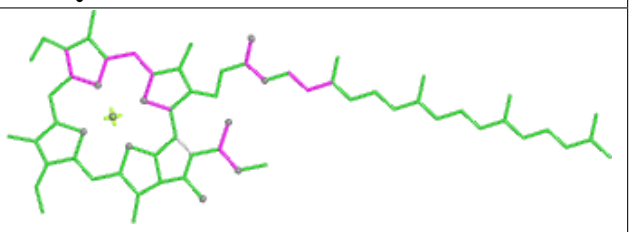
Ligand CLA n 611



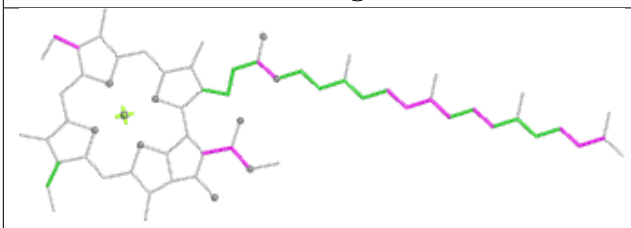
Ligand CLA BQ 603



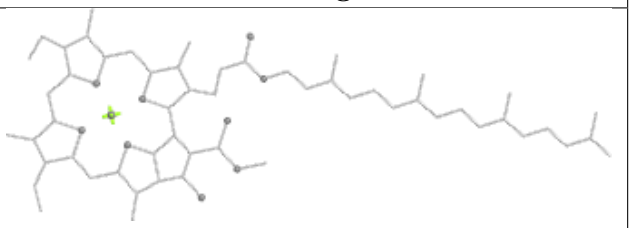
Bond lengths



Bond angles

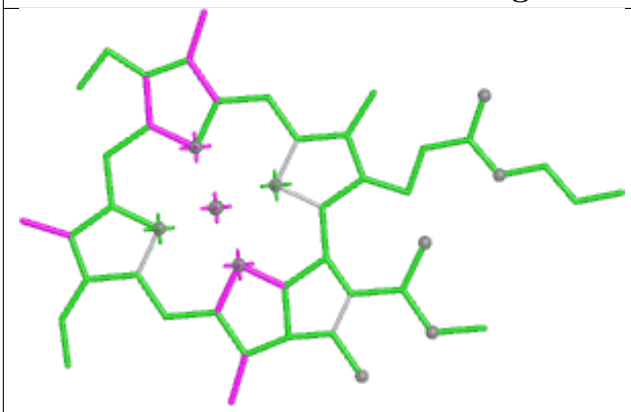


Torsions

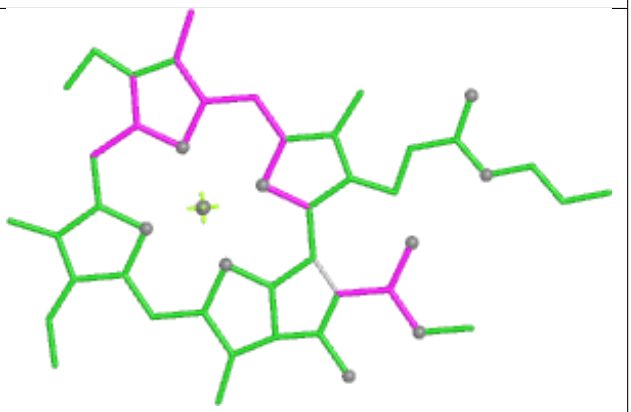


Rings

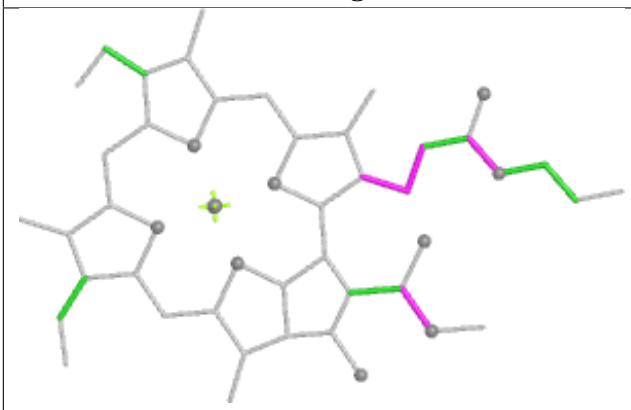
Ligand CLA BB 315



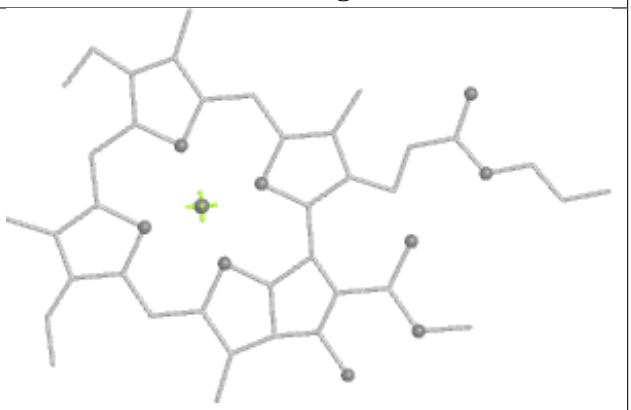
Bond lengths



Bond angles



Torsions



Rings

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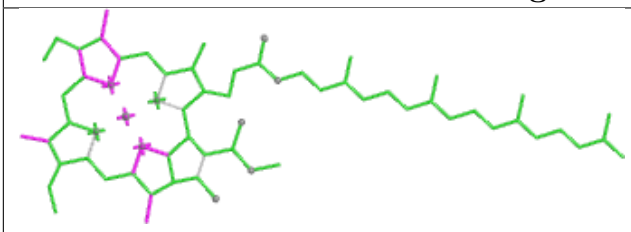
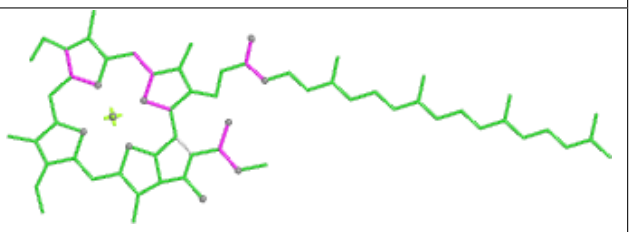
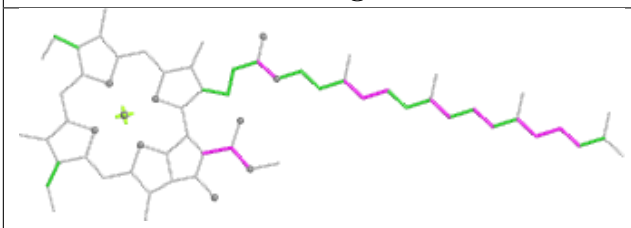
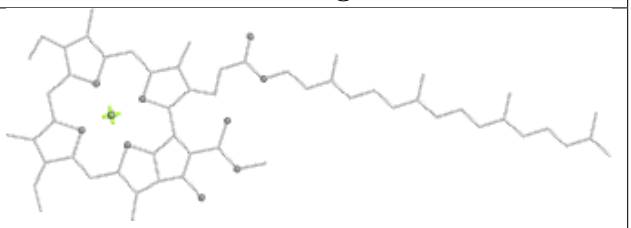
 Bond lengths	 Bond angles
 Torsions	 Rings

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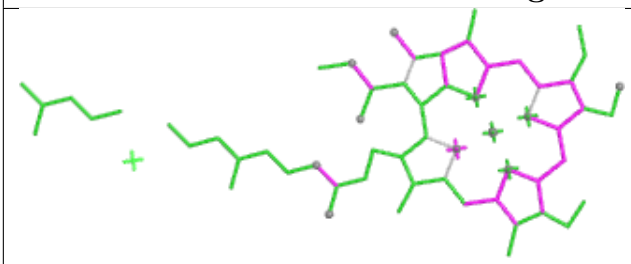
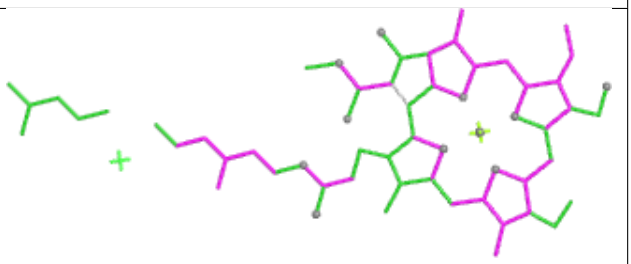
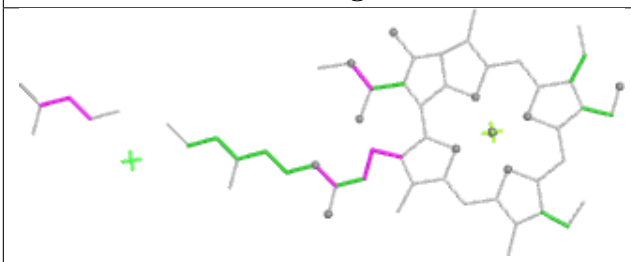
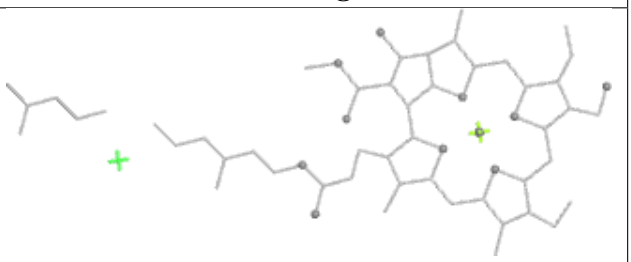
 Bond lengths	 Bond angles
 Torsions	 Rings

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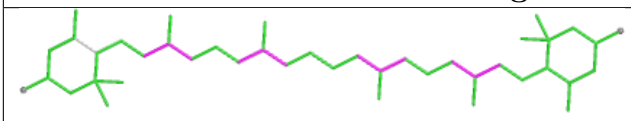
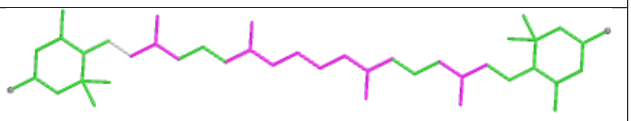
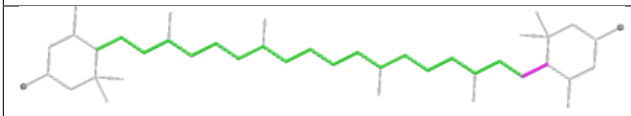
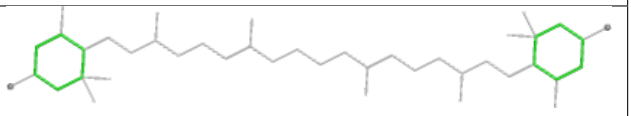
 Bond lengths	 Bond angles
 Torsions	 Rings

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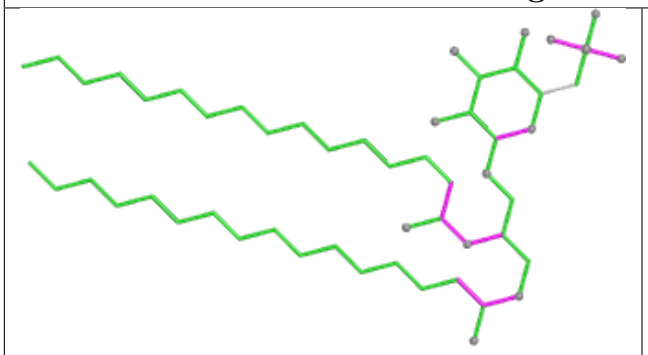

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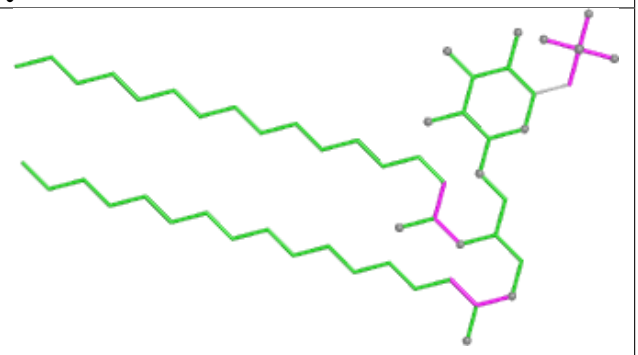

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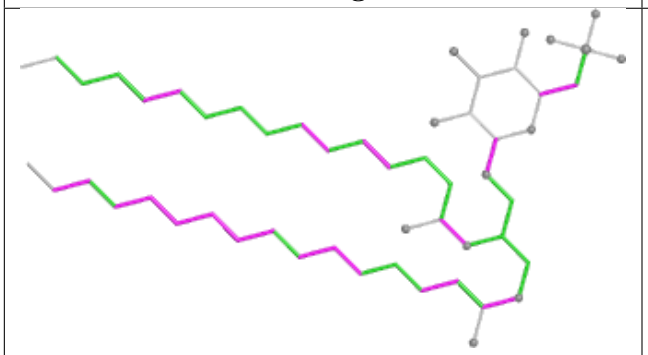

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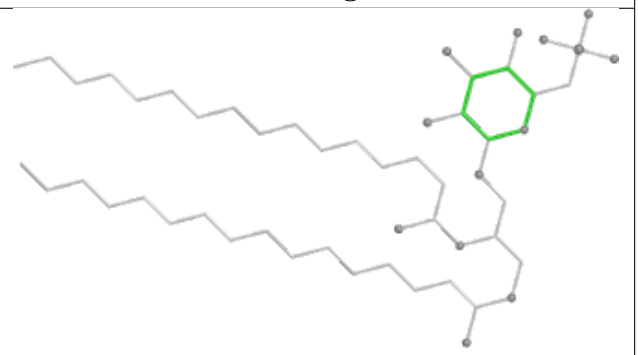
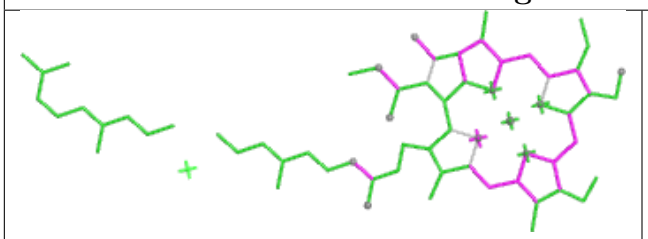


Rings

Ligand CHL Au 607



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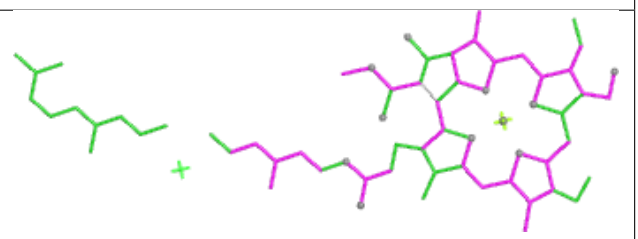

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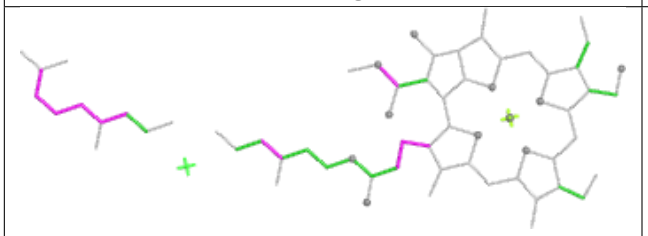

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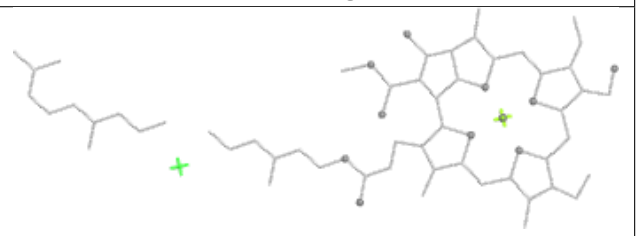

Rings

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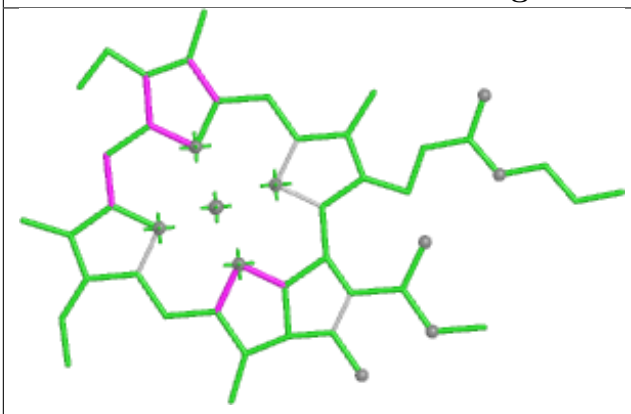
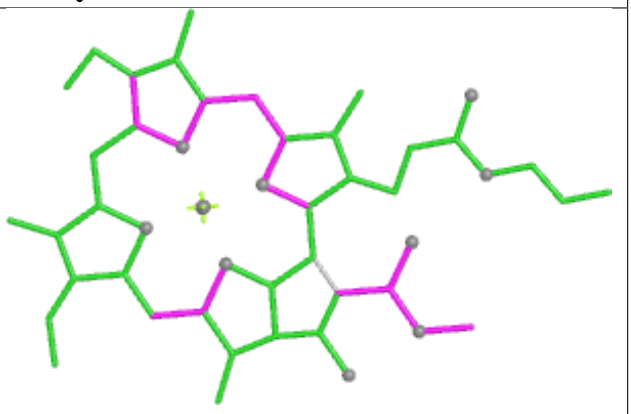
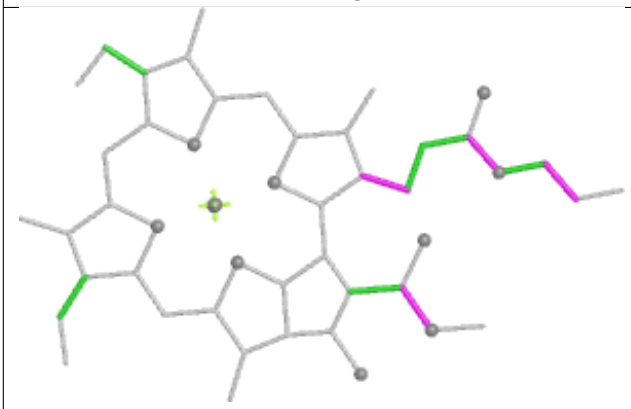
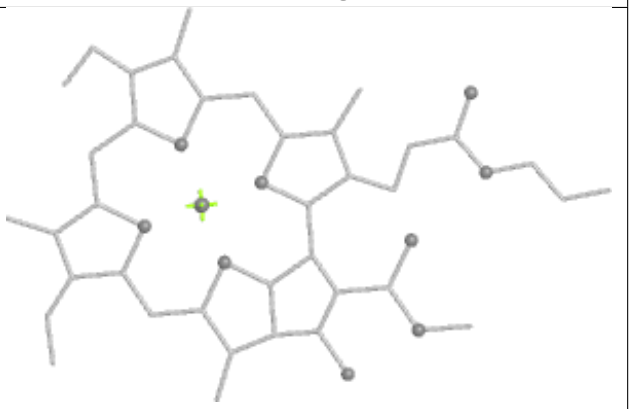
 Bond lengths	 Bond angles
 Torsions	 Rings

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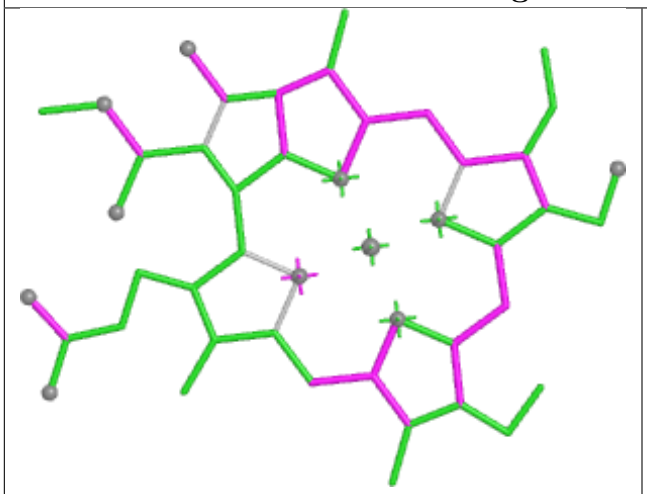

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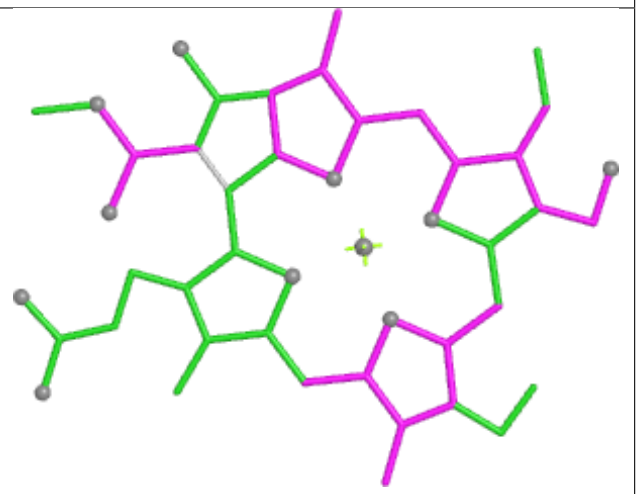

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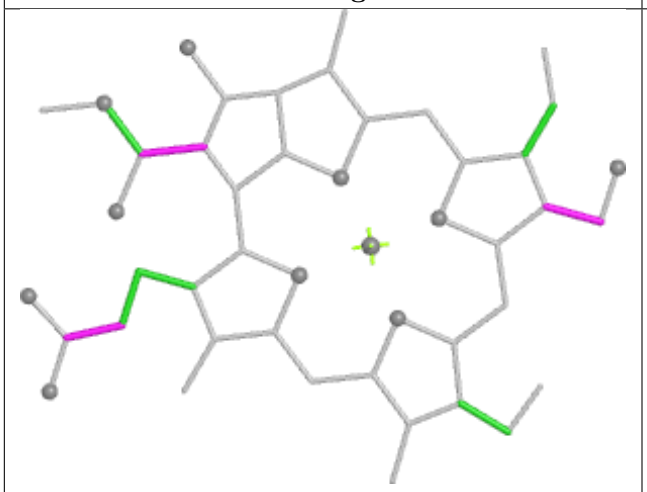

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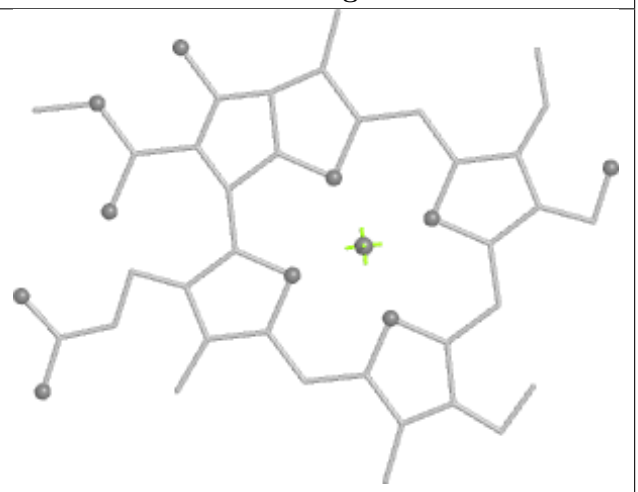

Rings

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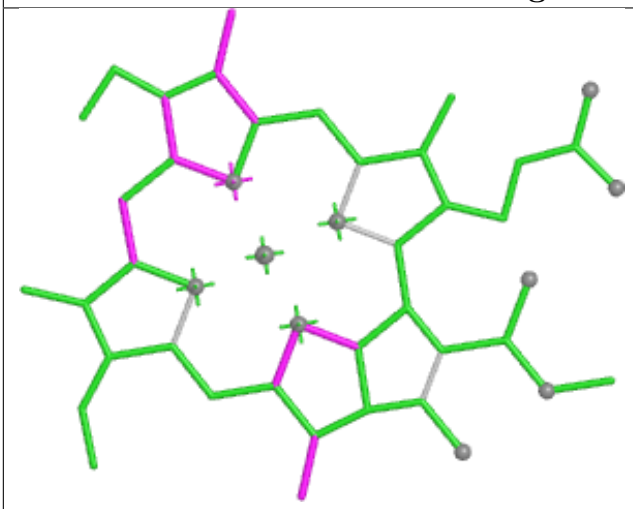

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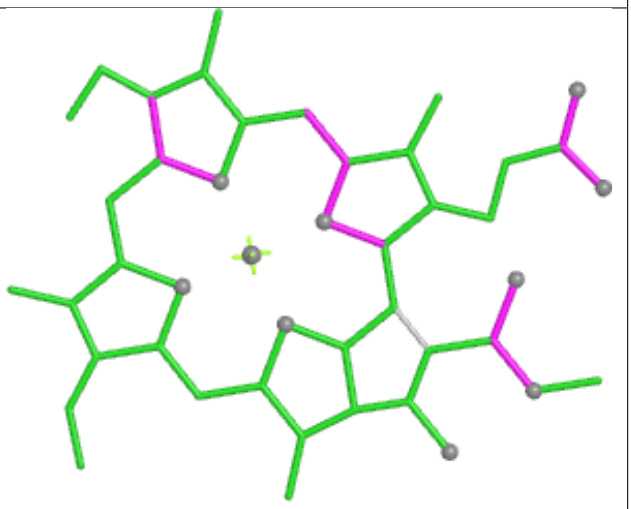

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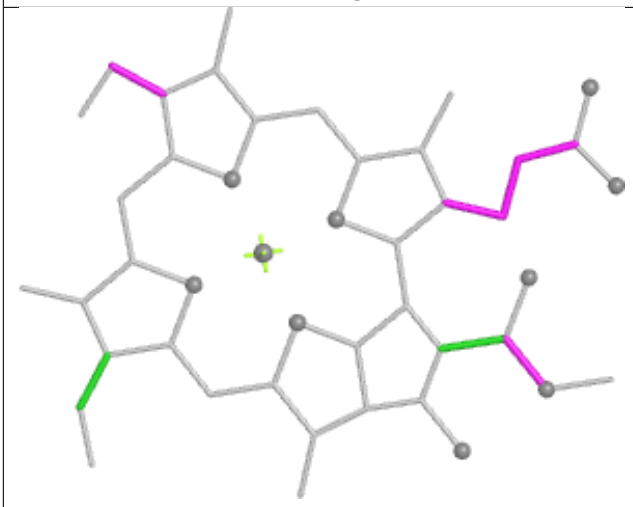

Torsions

Rings

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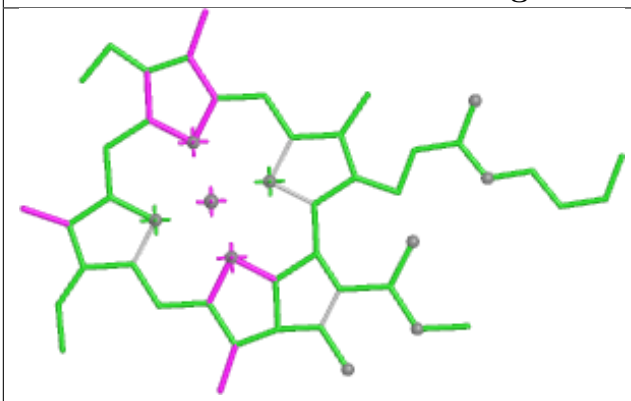

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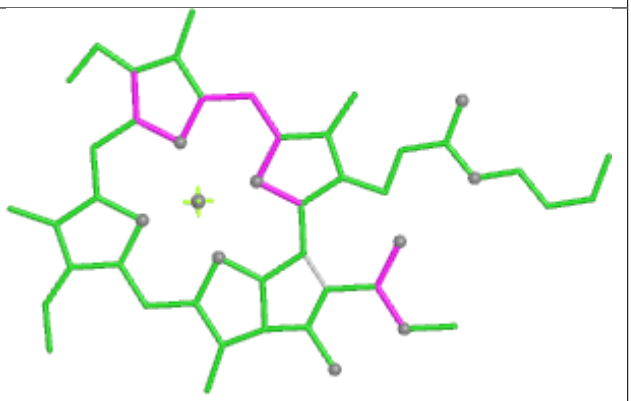

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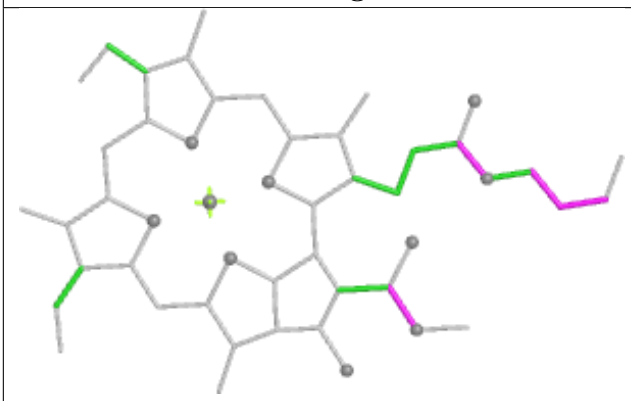

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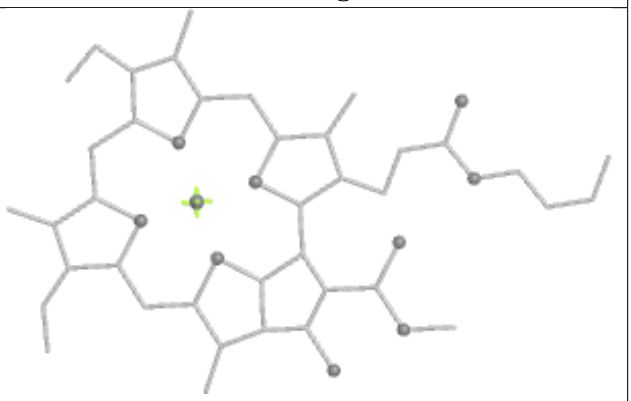

Rings

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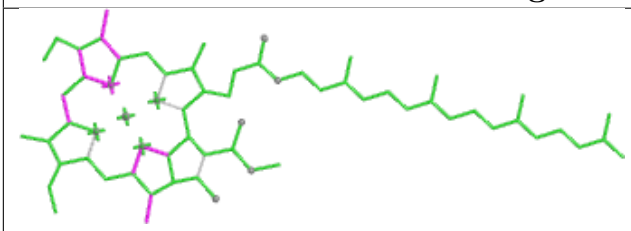

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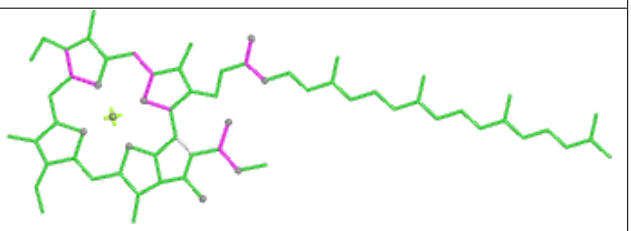

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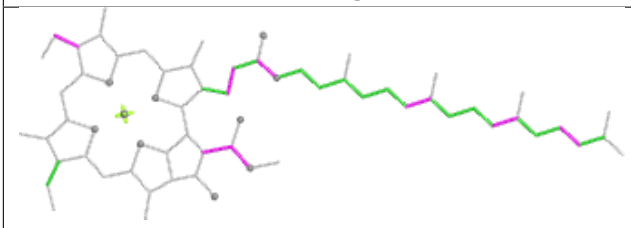

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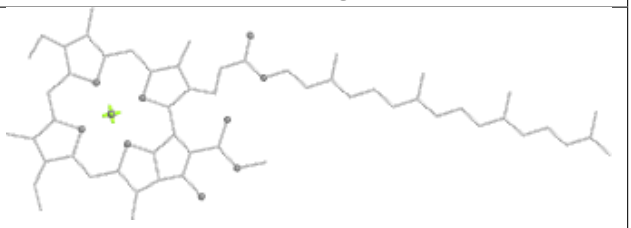

Rings

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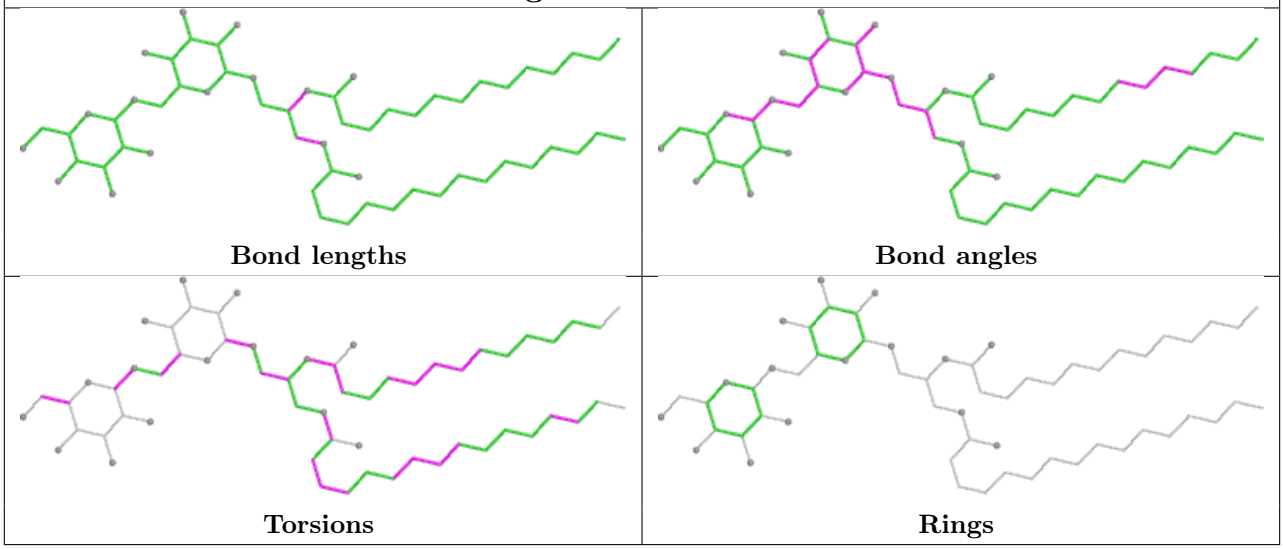

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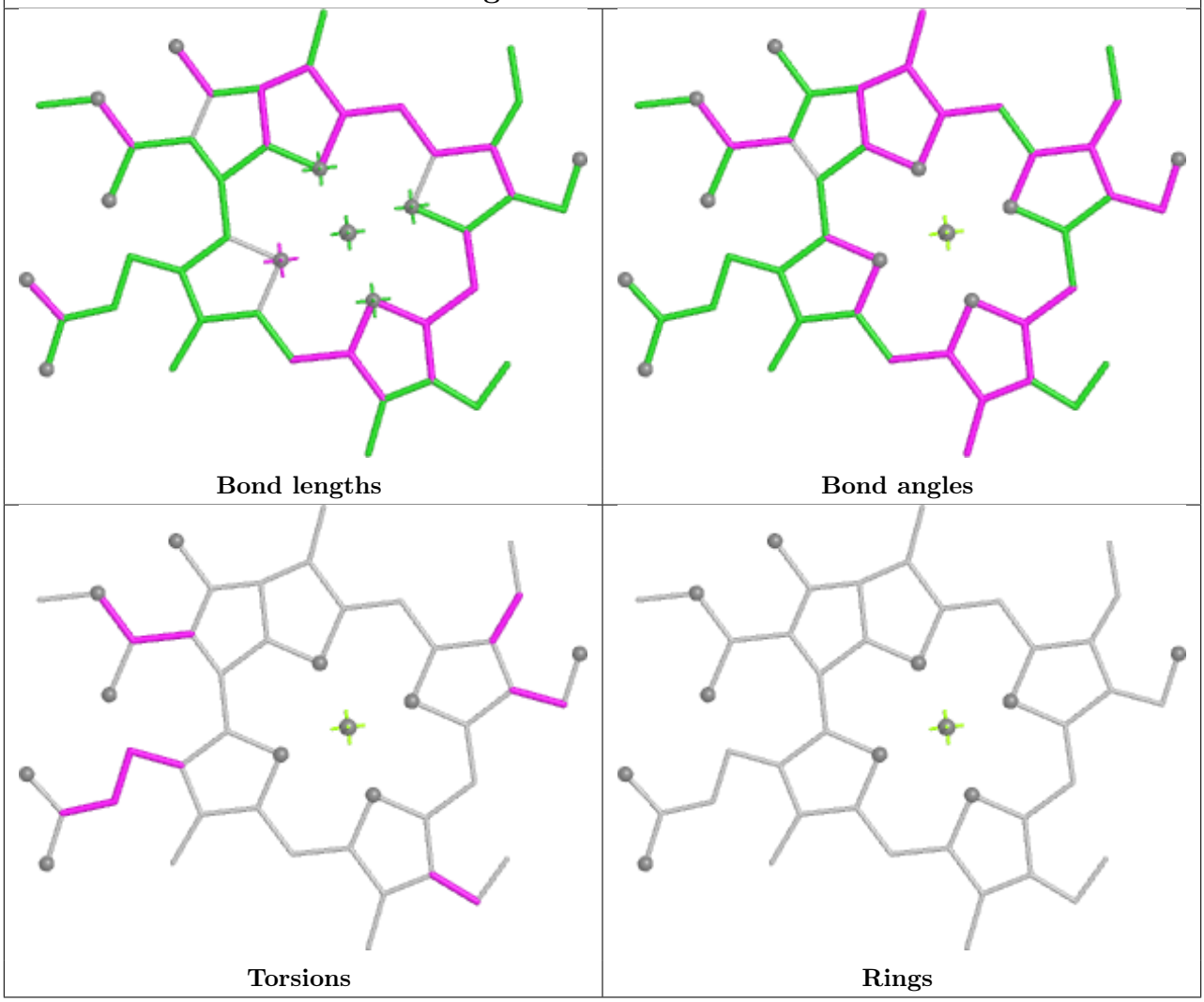

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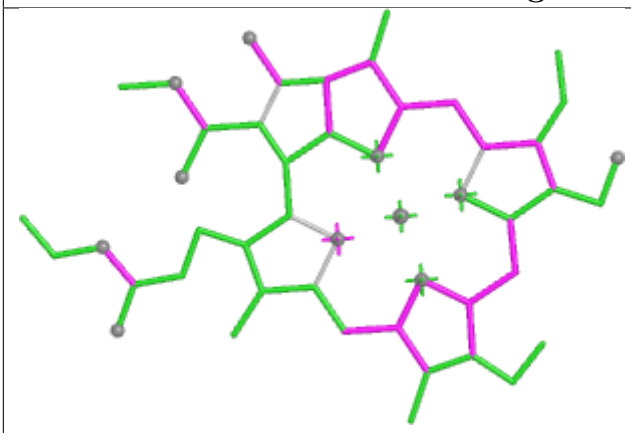
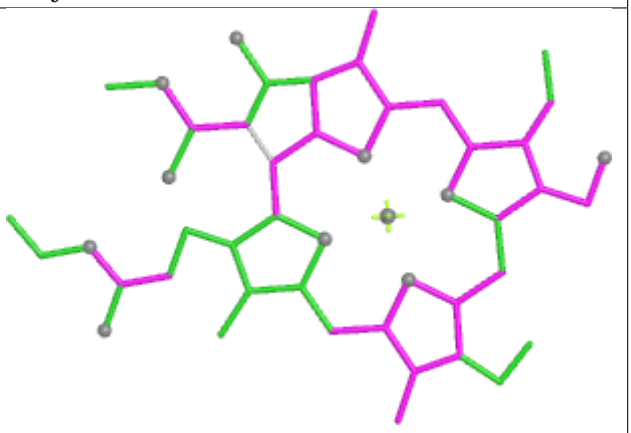
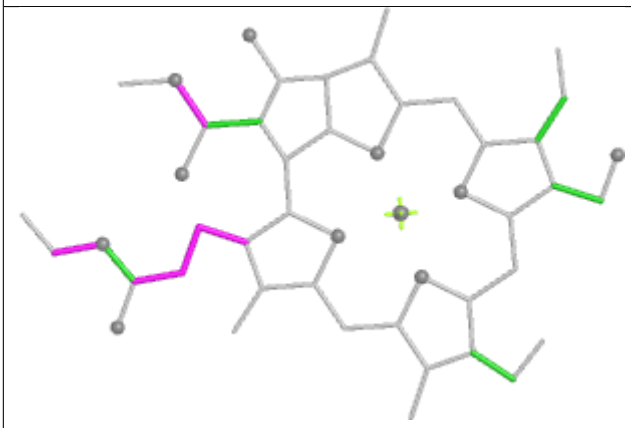
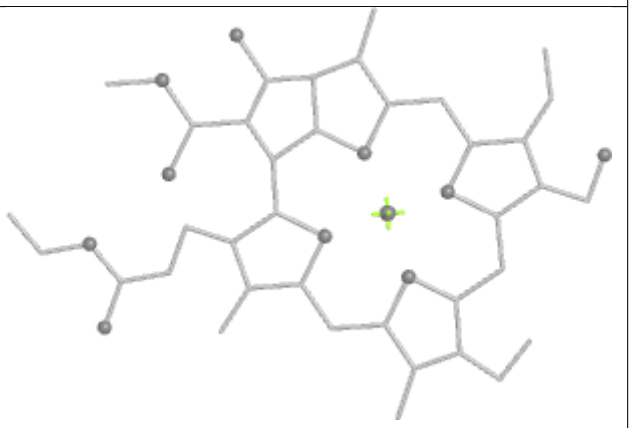
 Bond lengths	 Bond angles
 Torsions	 Rings

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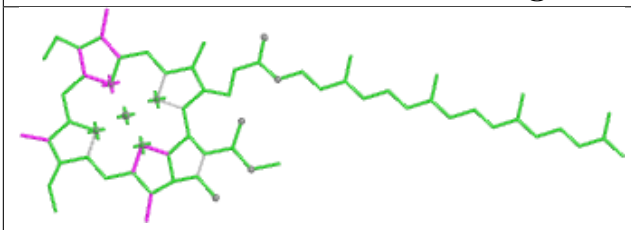
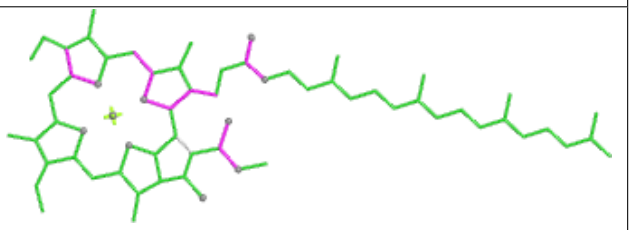
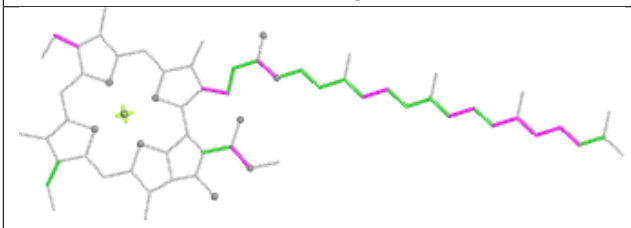
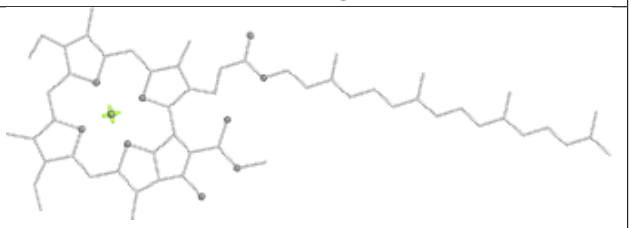
 Bond lengths	 Bond angles
 Torsions	 Rings

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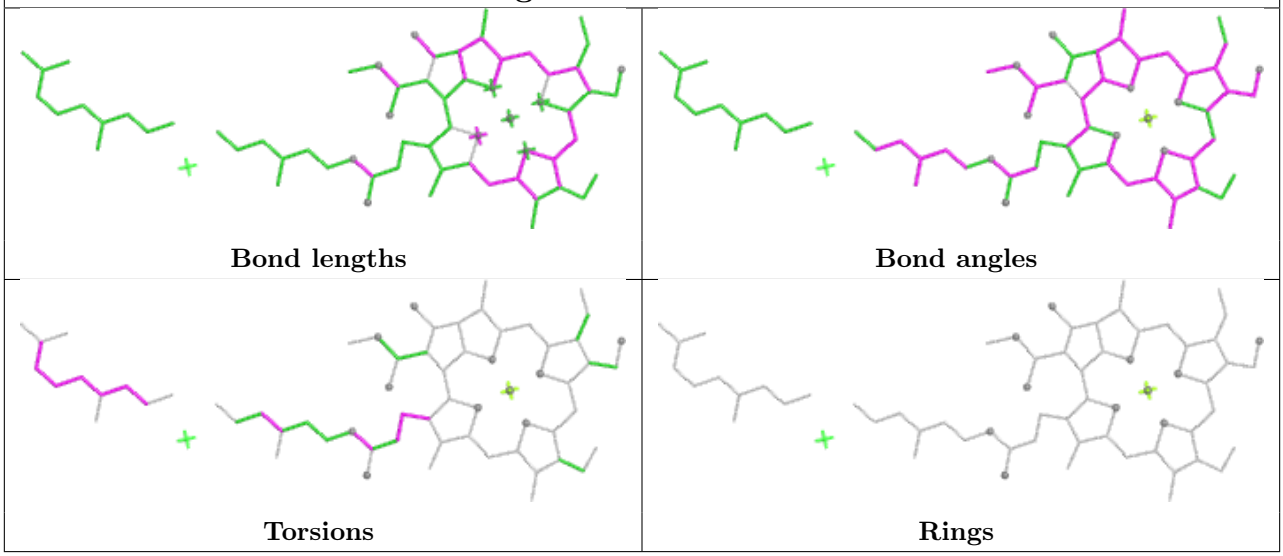

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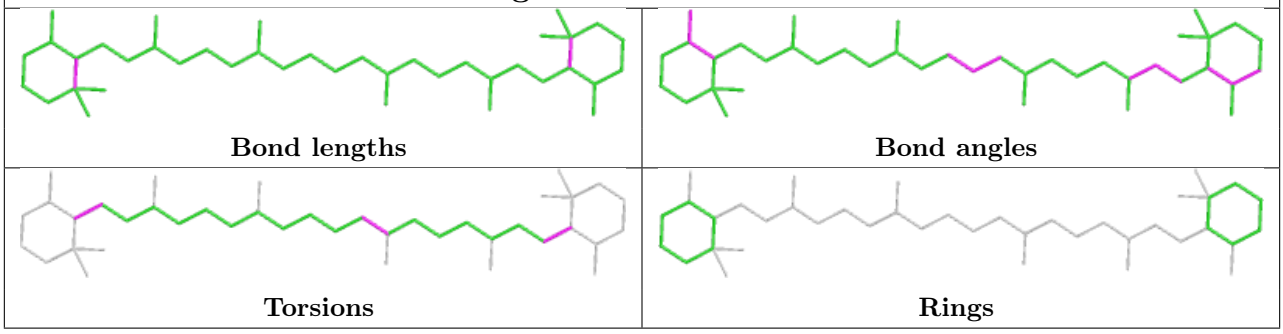

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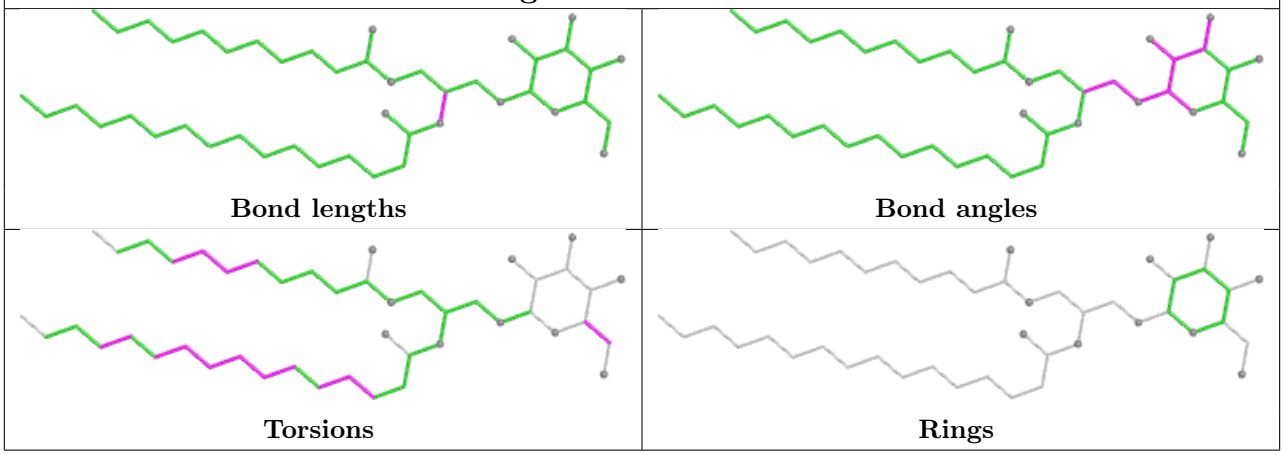

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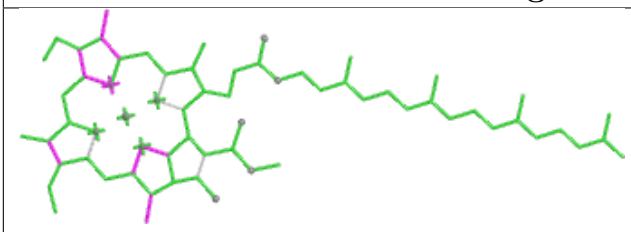
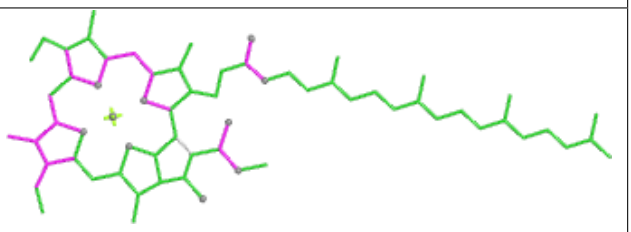
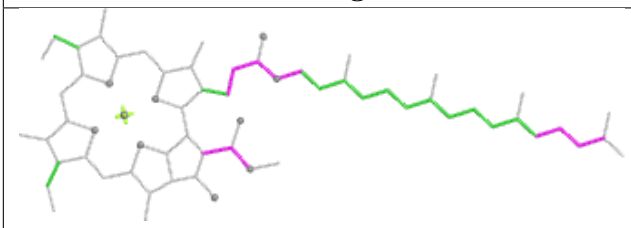
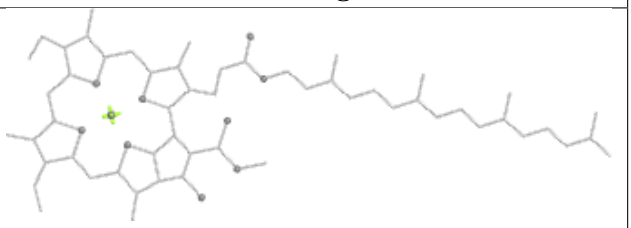
 Bond lengths	 Bond angles
 Torsions	 Rings

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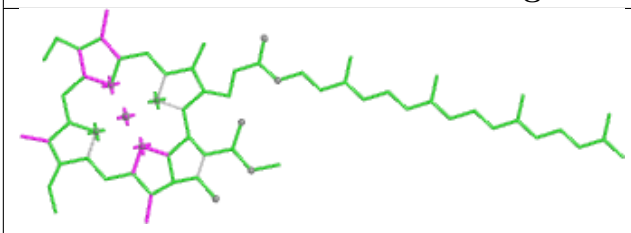
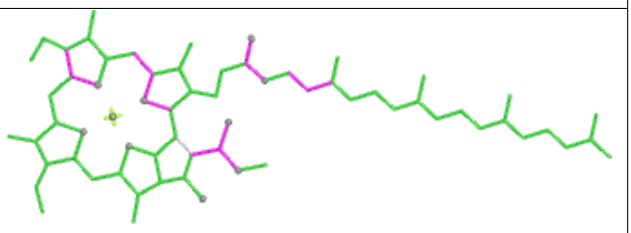
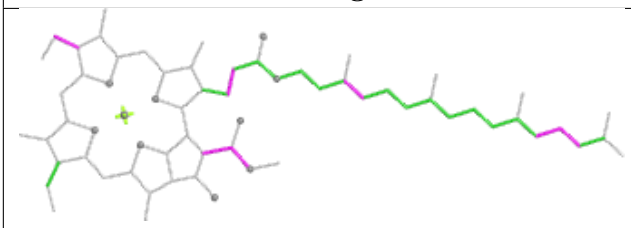
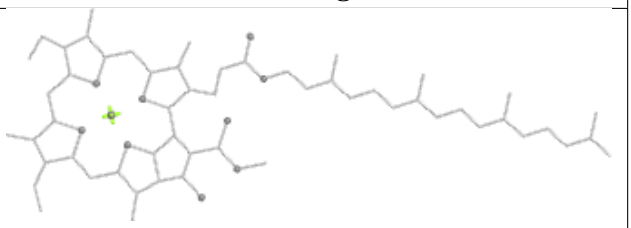
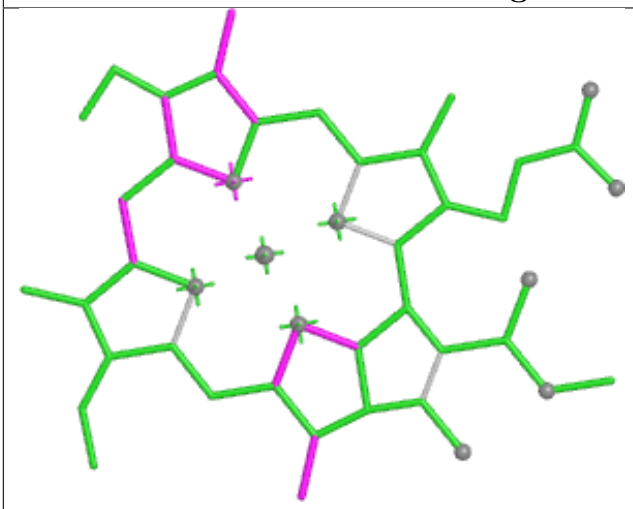
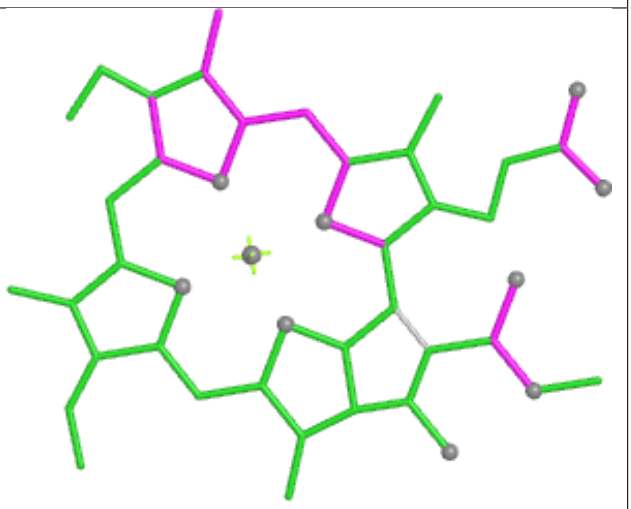
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 313



Bond lengths



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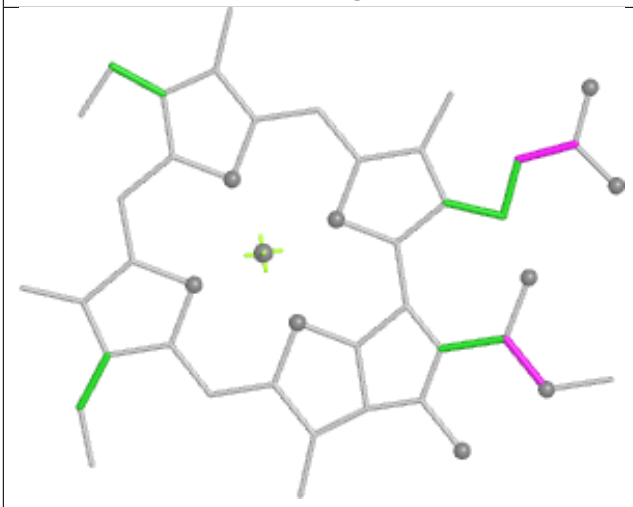
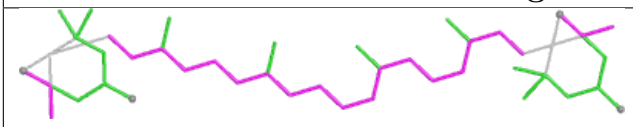


Torsions

Rings

Ligand XAT 7 301



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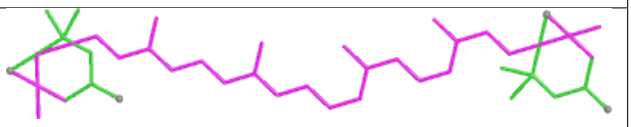

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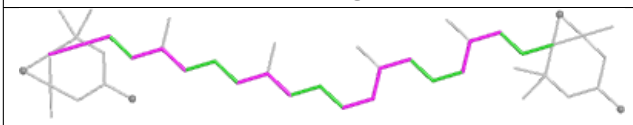

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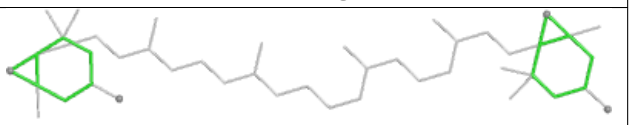
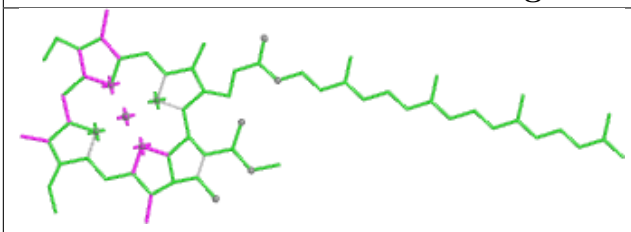
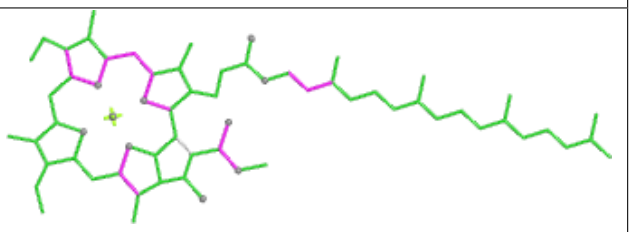
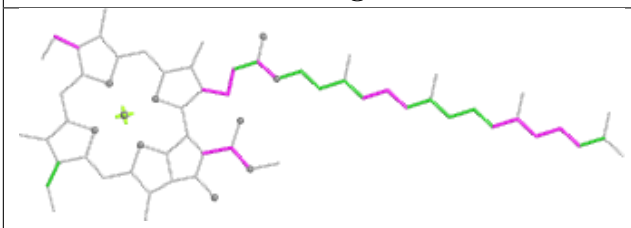
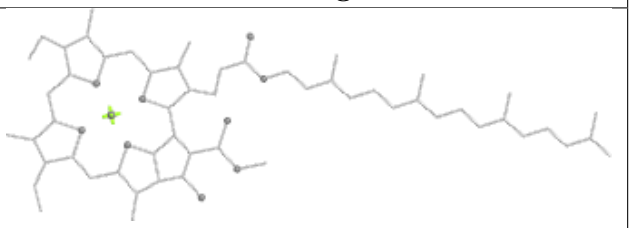
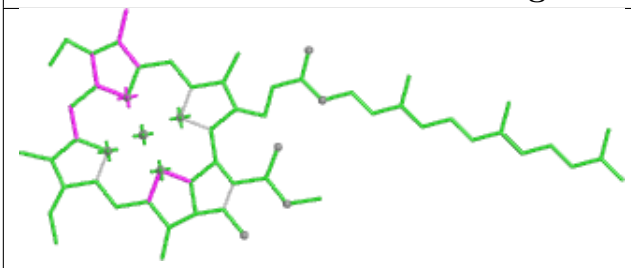
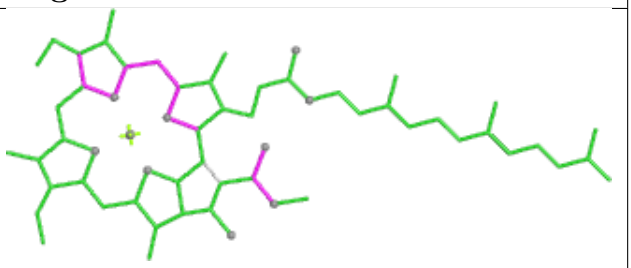
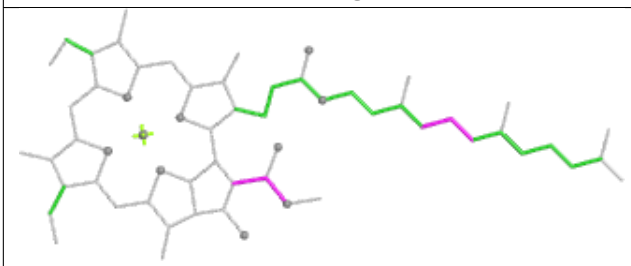
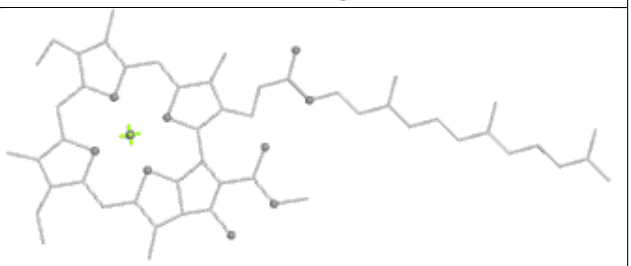
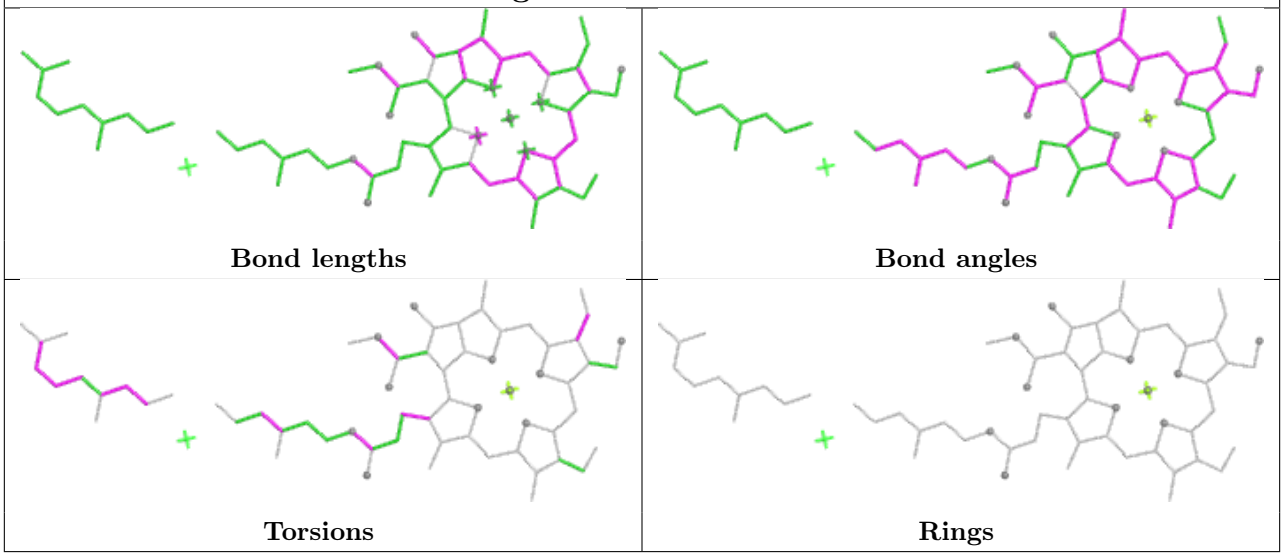


Rings

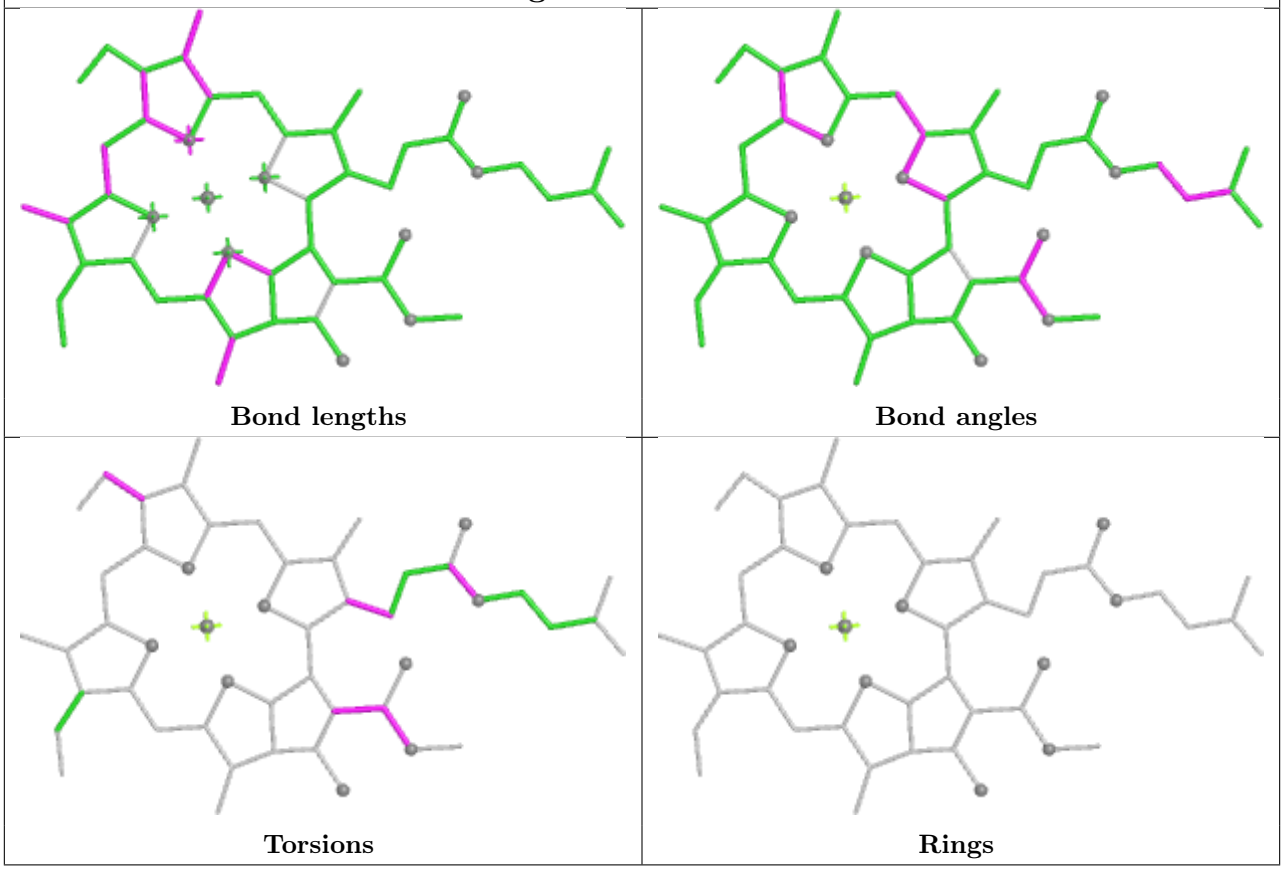
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL BB 302



Ligand CLA S 604



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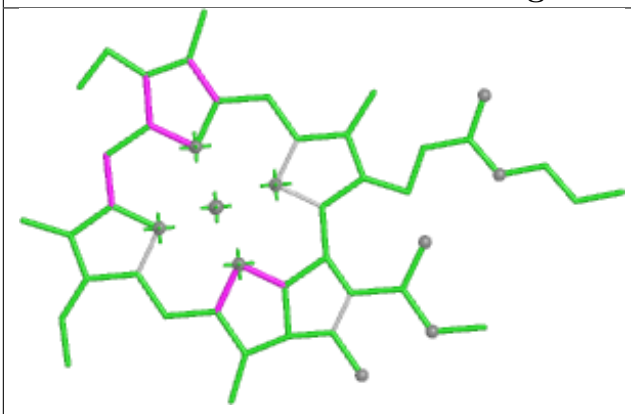
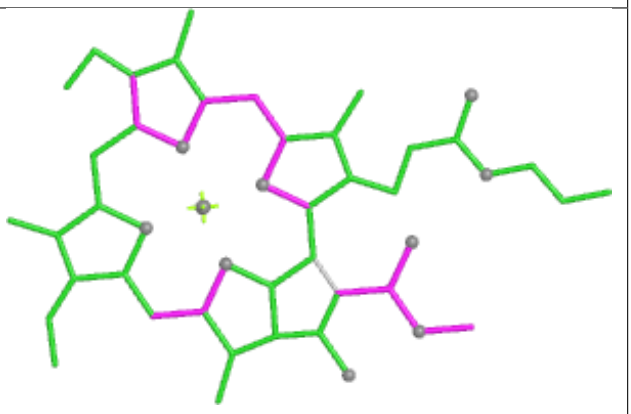
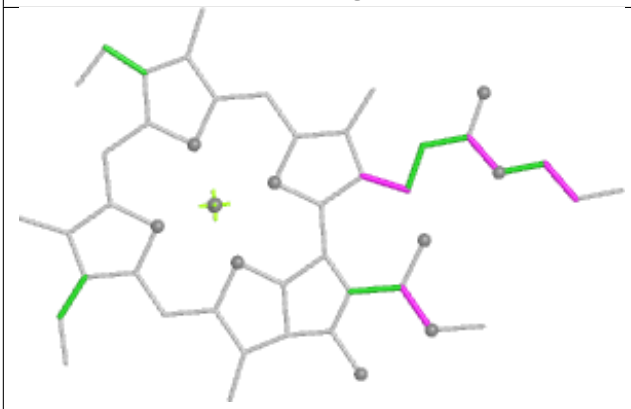
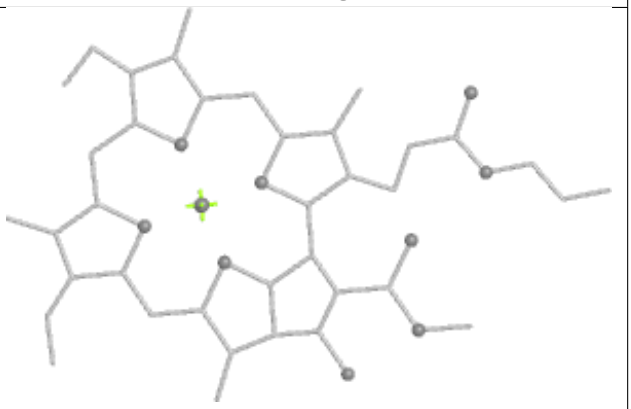
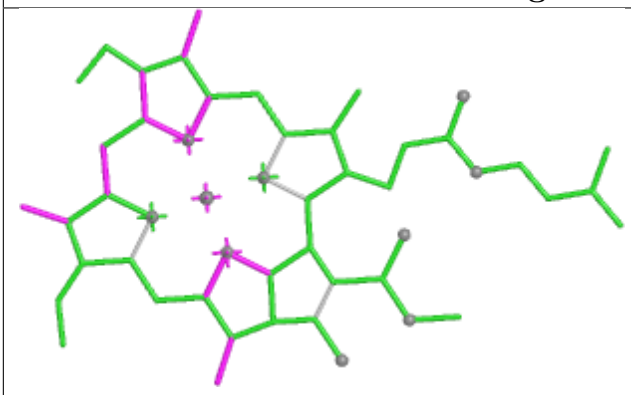
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 604



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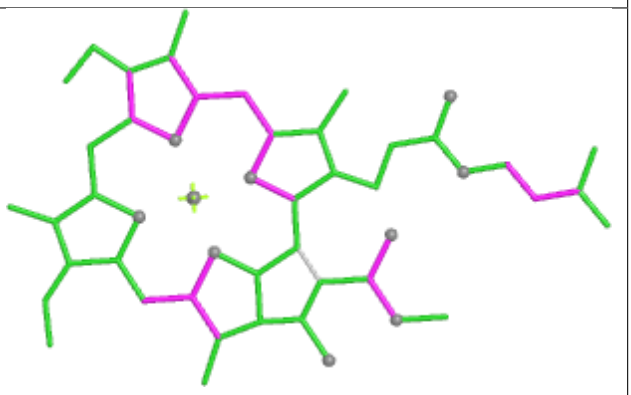
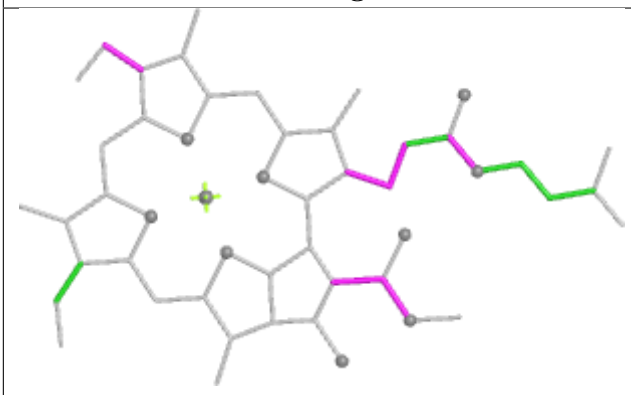


Bond angles



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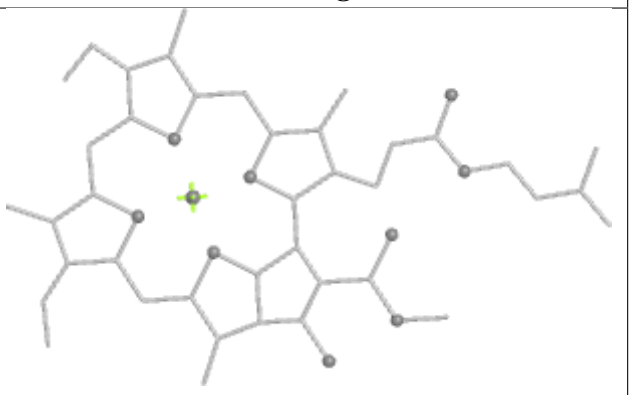
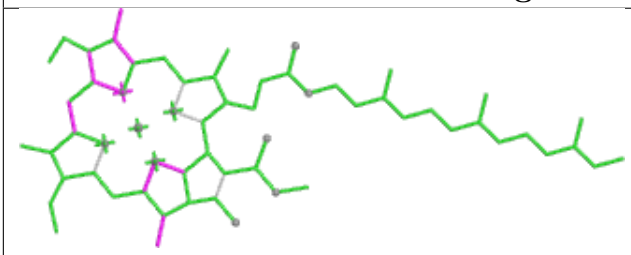


Rings

Ligand CLA A6 602



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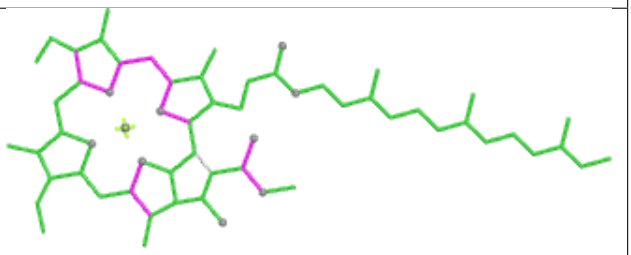

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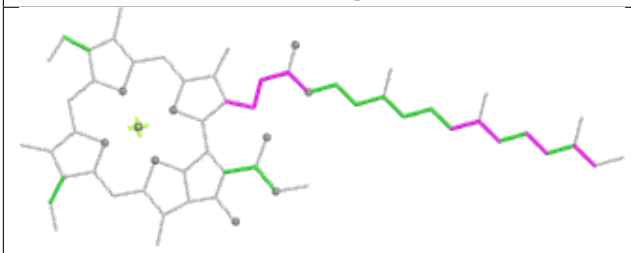

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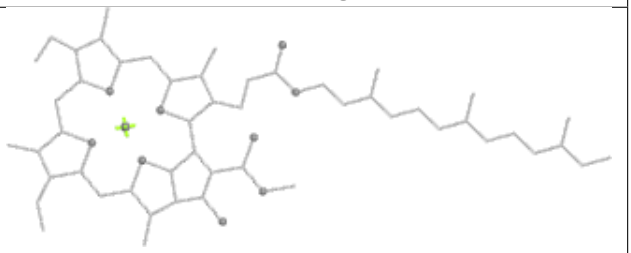
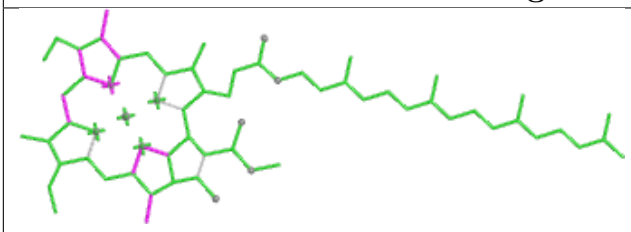
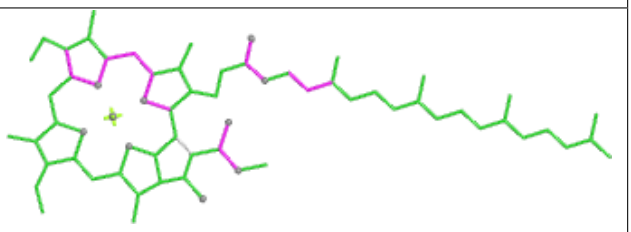
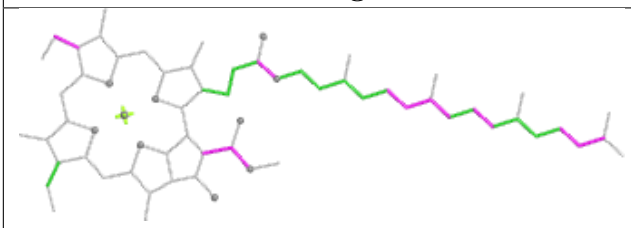
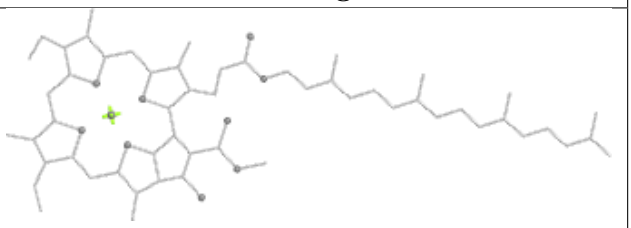


Rings

Ligand CLA n 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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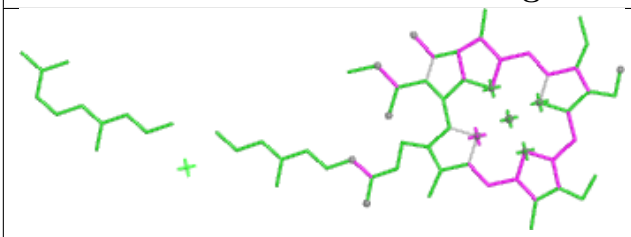
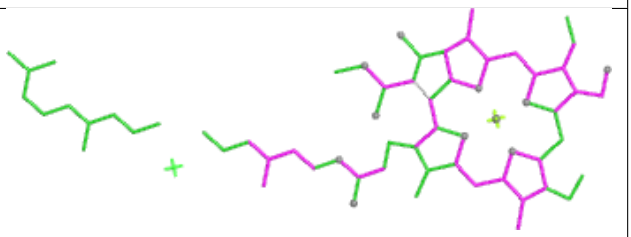
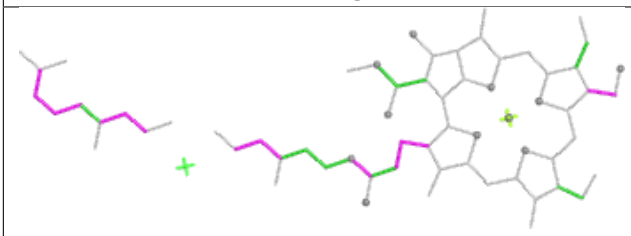
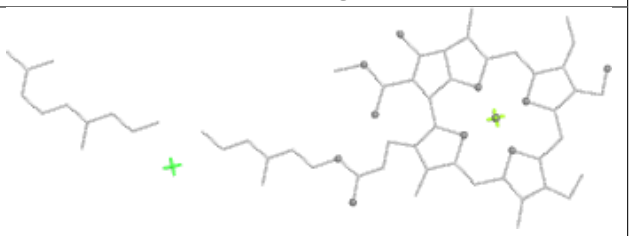
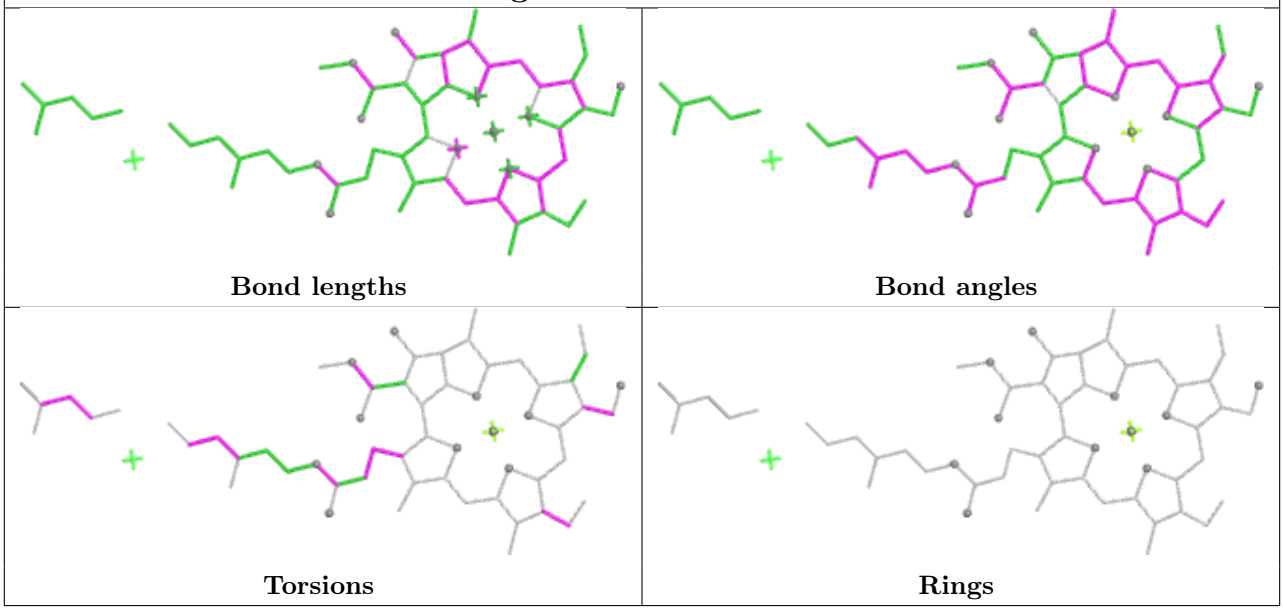
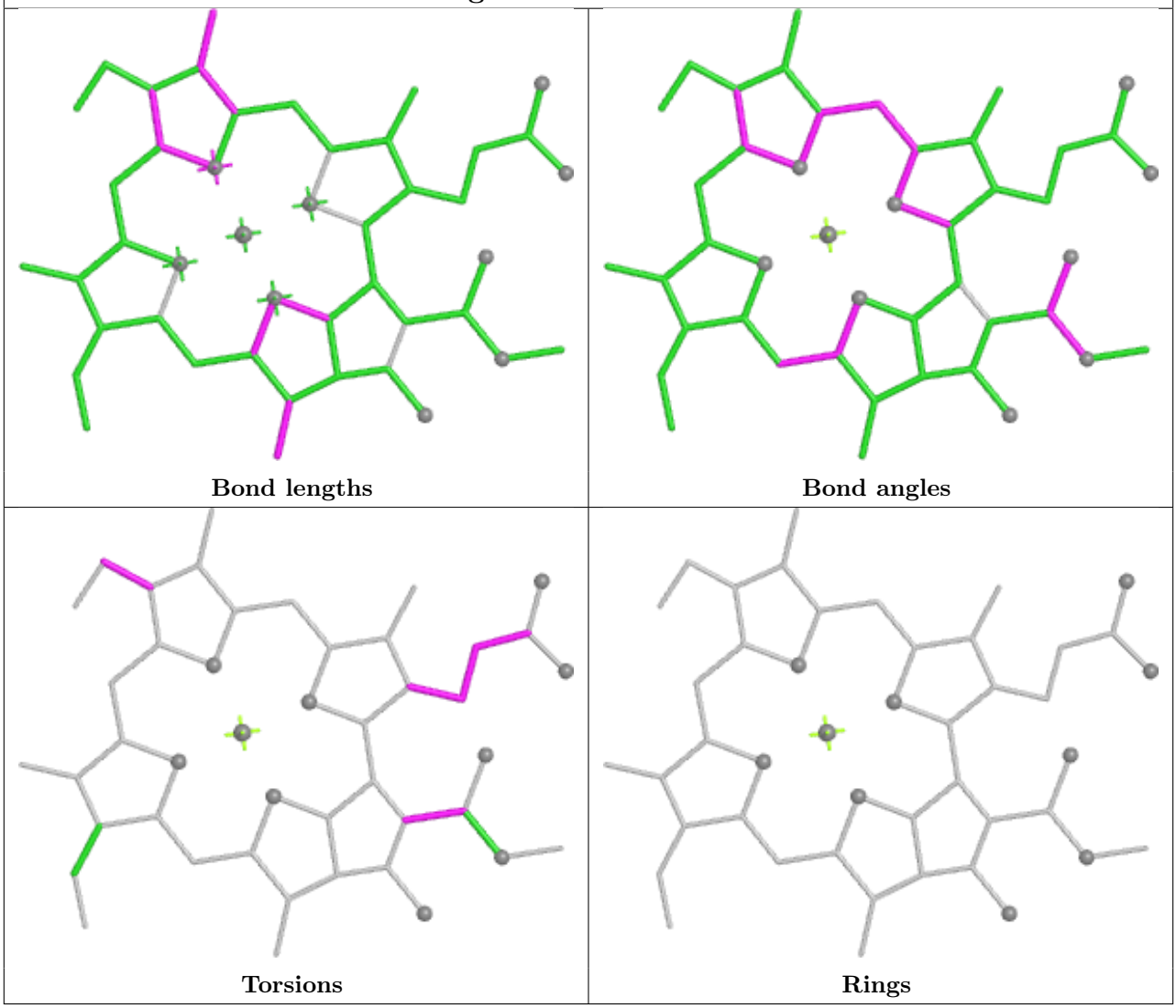
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AA 308



Ligand CLA AA 312



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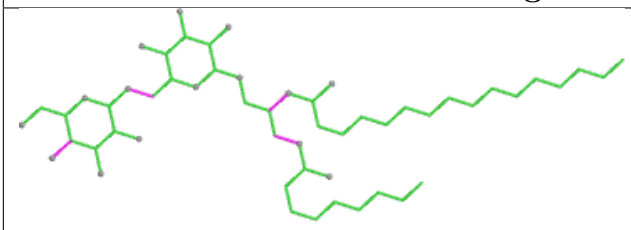
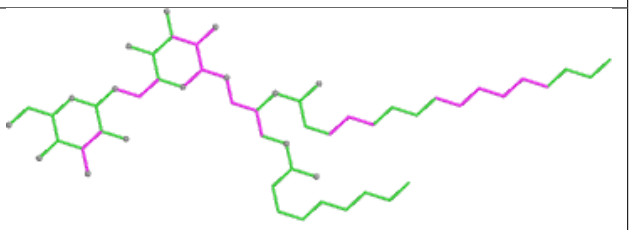
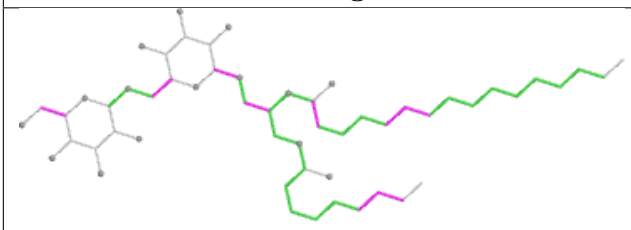
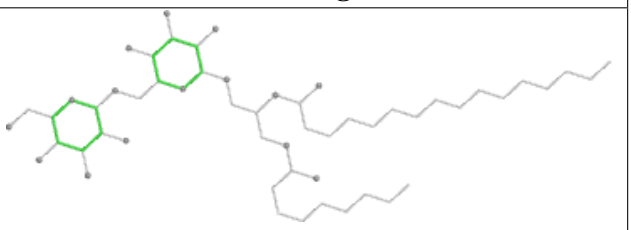
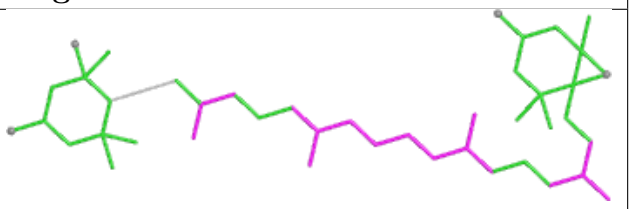
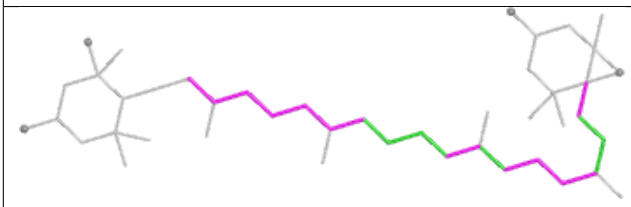
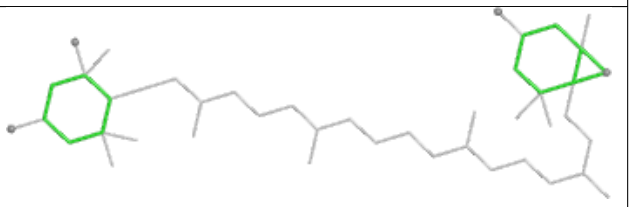
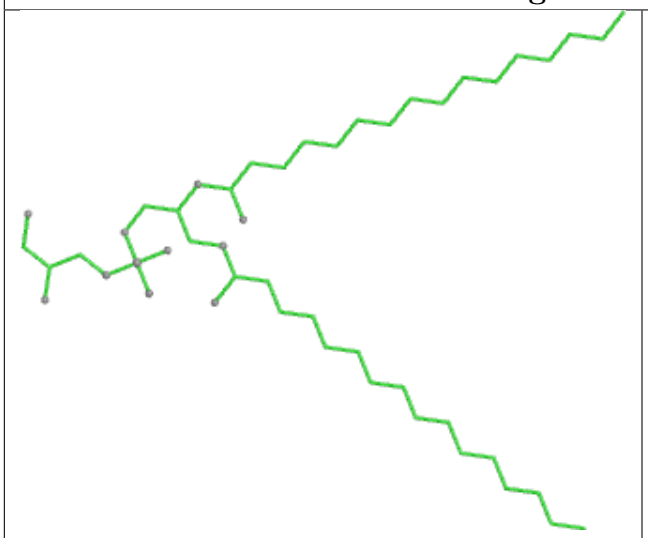
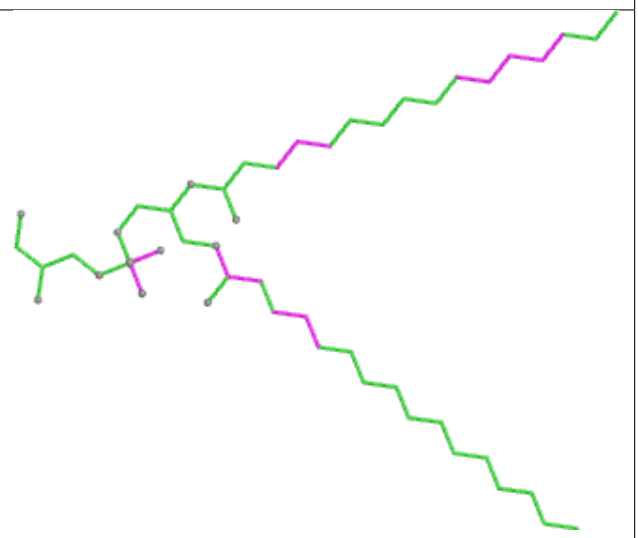
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX g 617	
Bond lengths	 Bond angles
 Torsions	 Rings

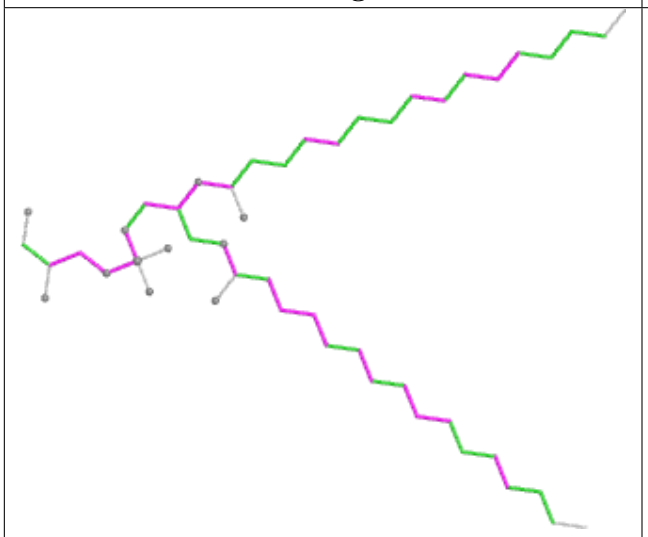
Ligand LHG c 519



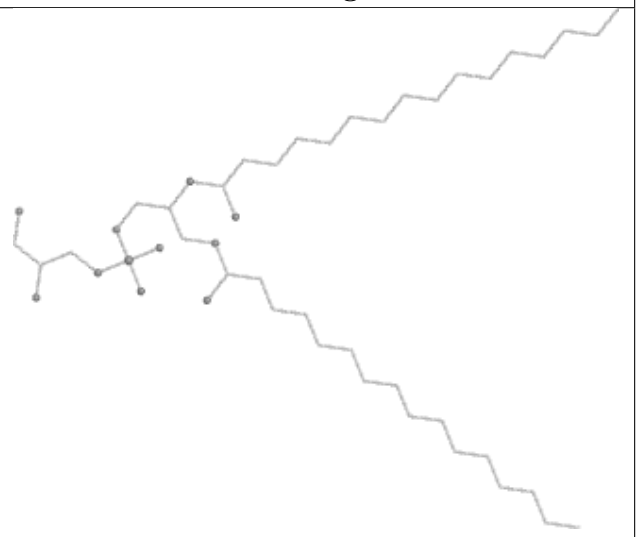
Bond lengths



Bond angles

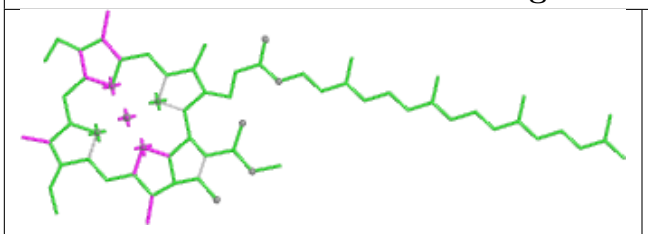


Torsions

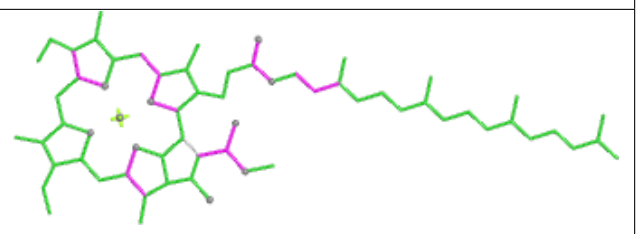


Rings

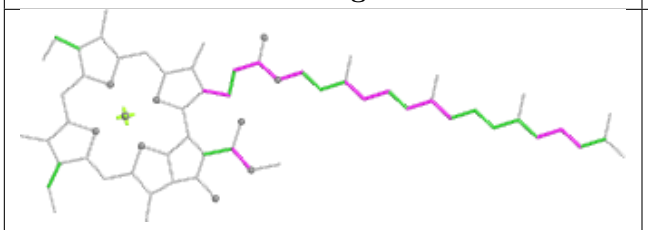
Ligand CLA 2 402



Bond lengths



Bond angles



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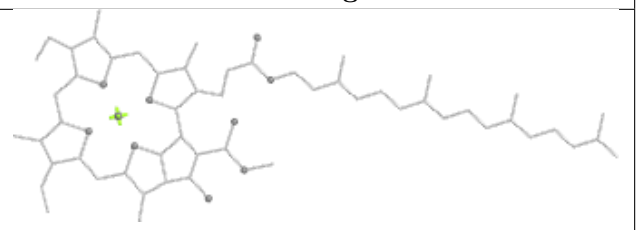
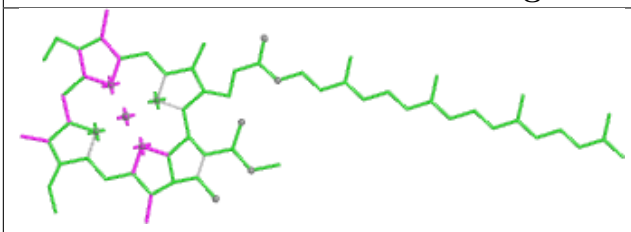
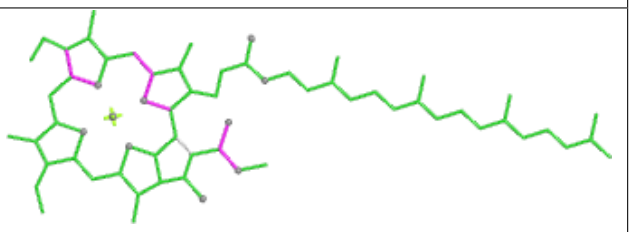
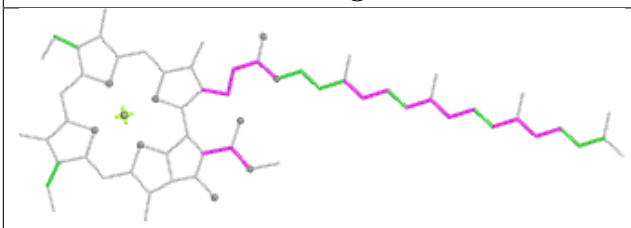
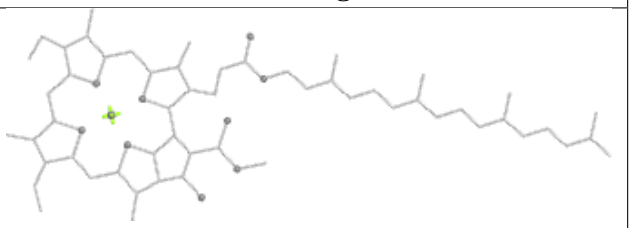
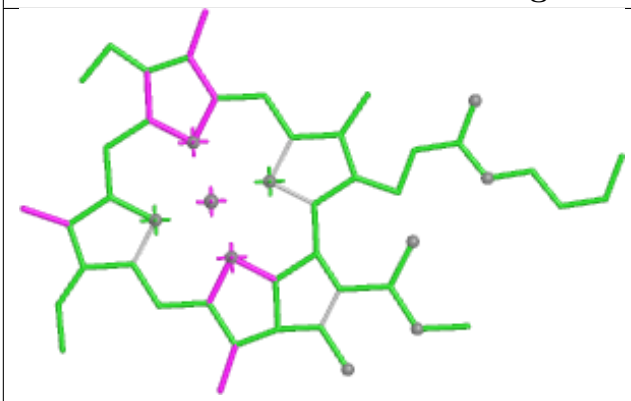
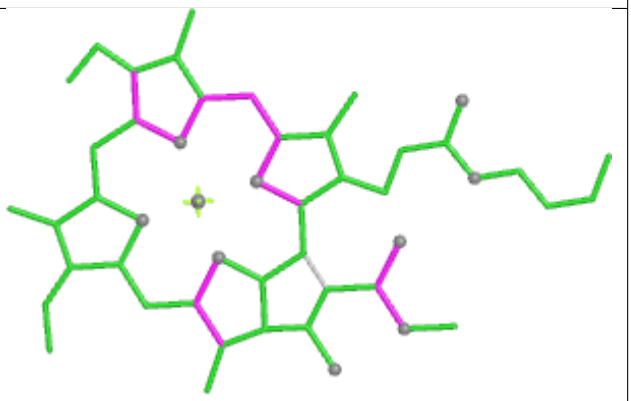
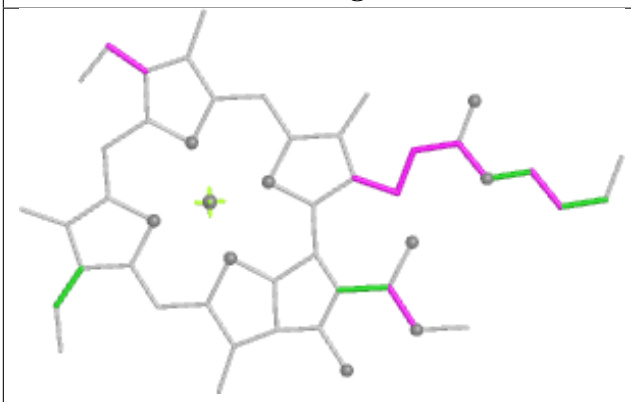
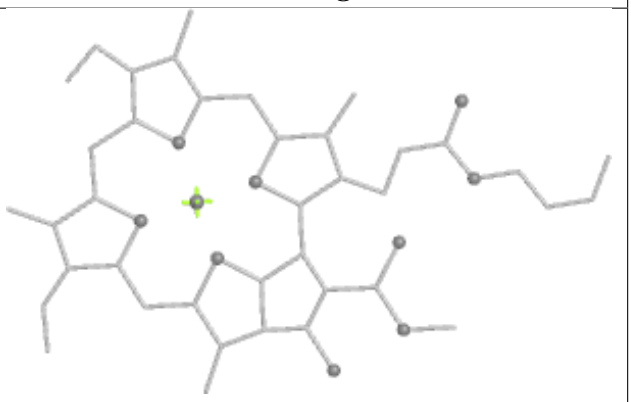
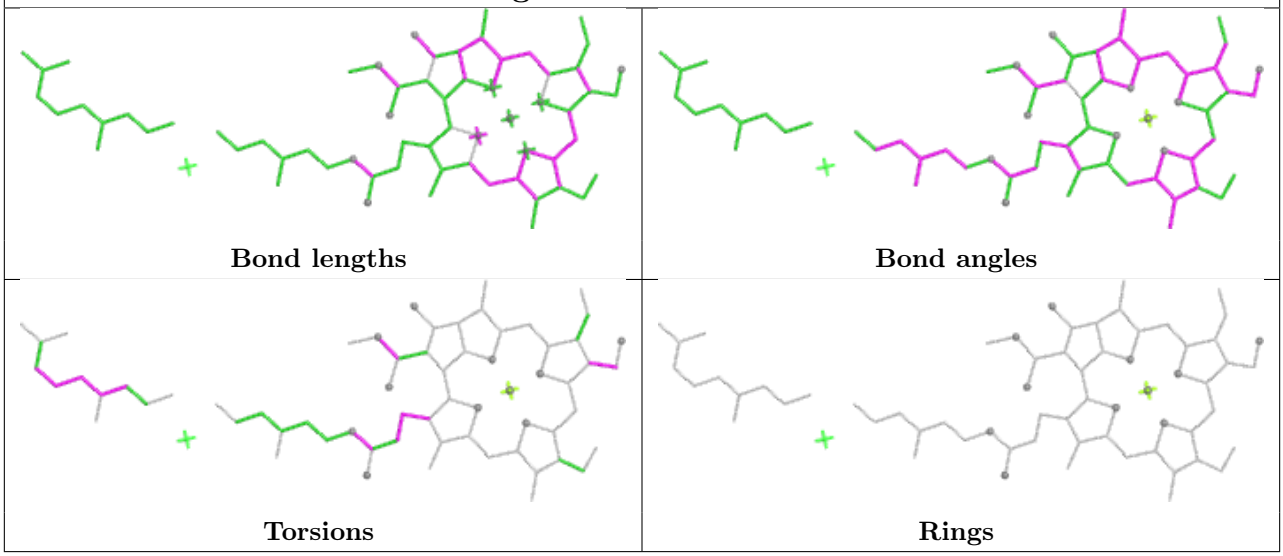


Rings

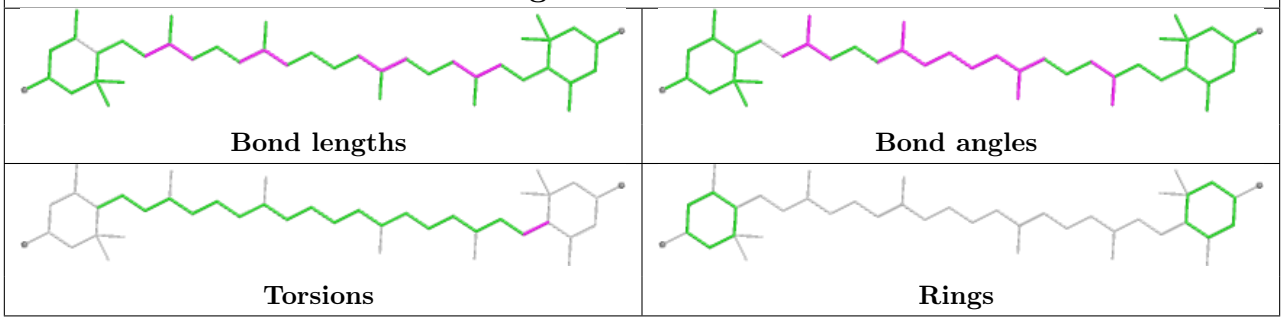
Ligand CLA Y 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

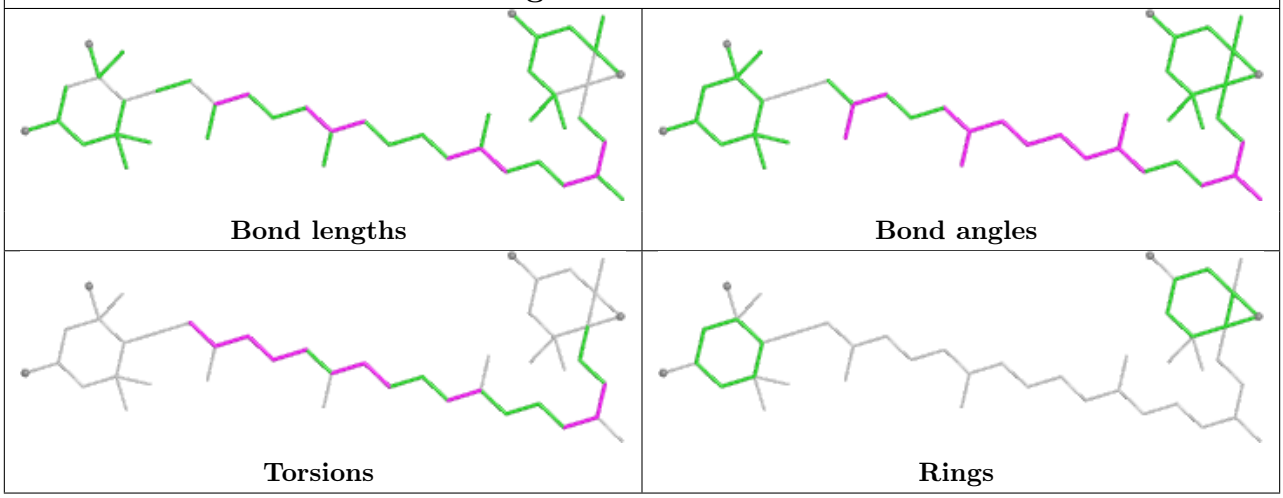
Ligand CHL BB 309



Ligand LUT 7 317



Ligand NEX S 616



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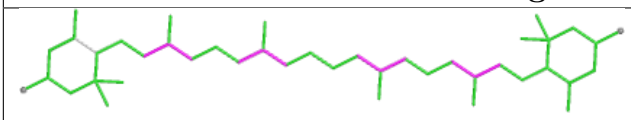
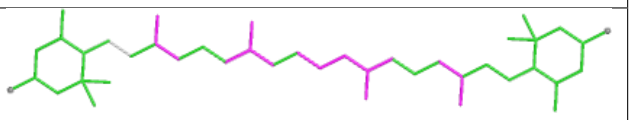
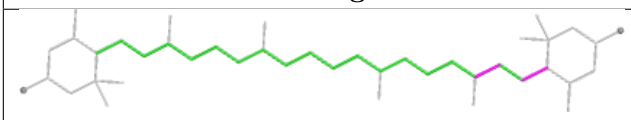


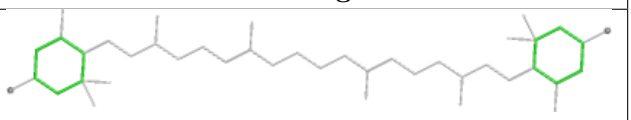
Bond lengths



Bond angles

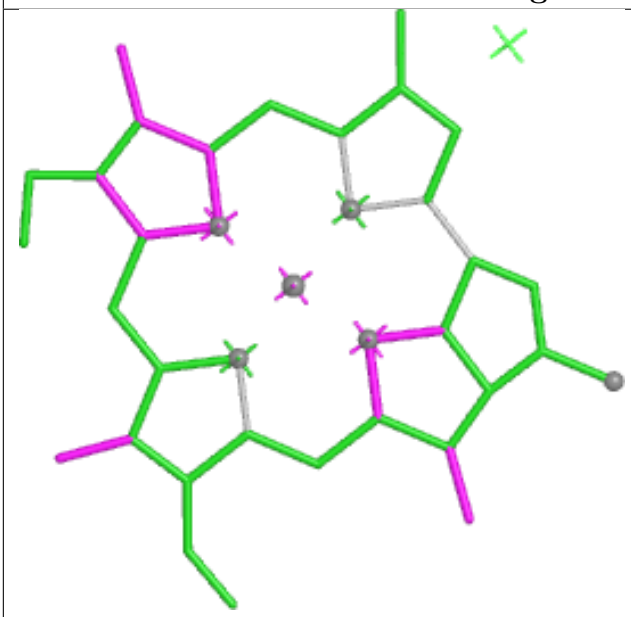


Torsions

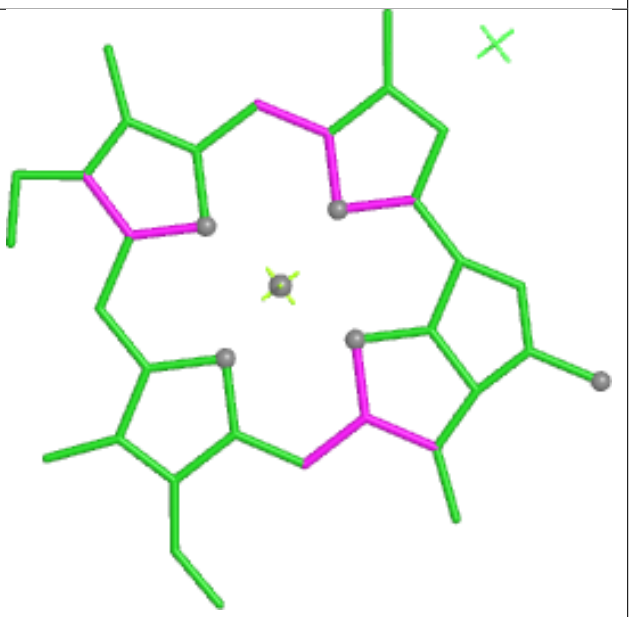


Rings

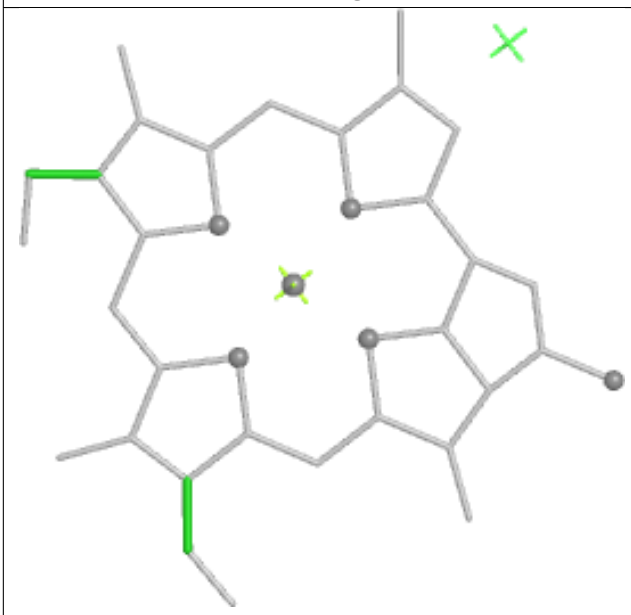
Ligand CLA r 612



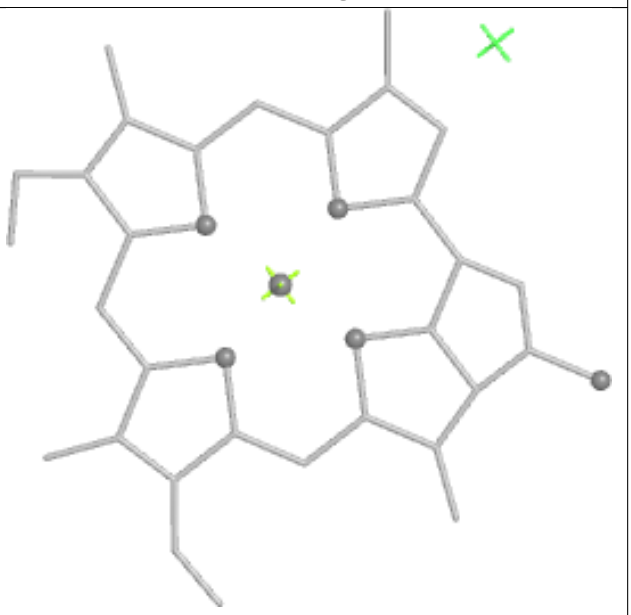
Bond lengths



Bond angles

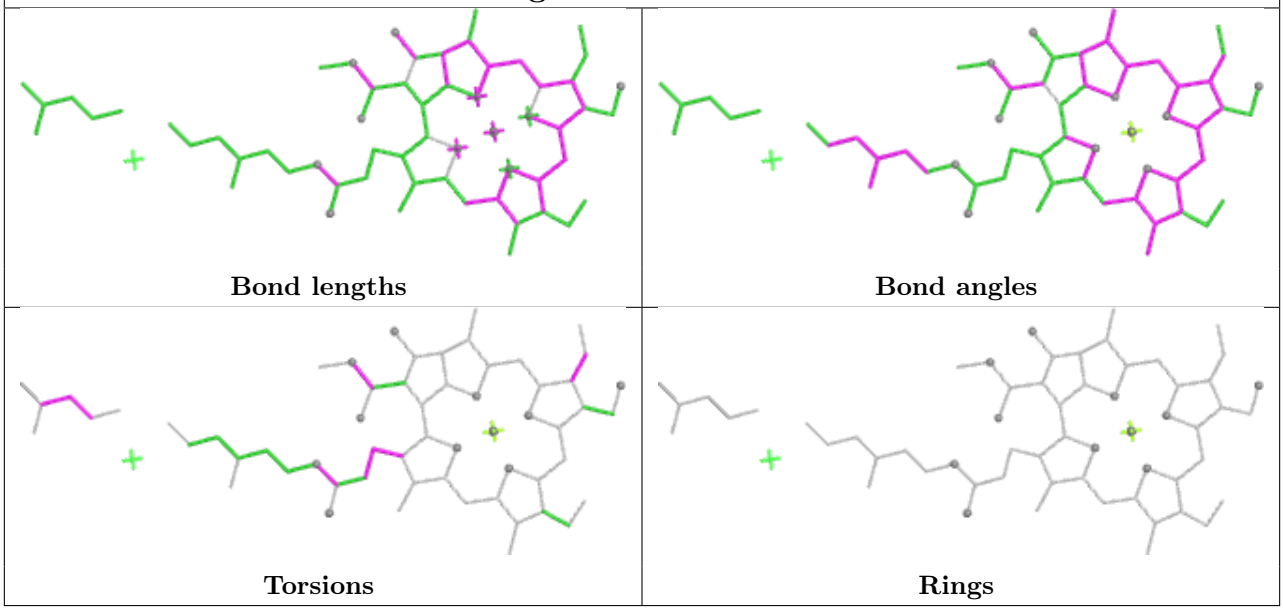


Torsions

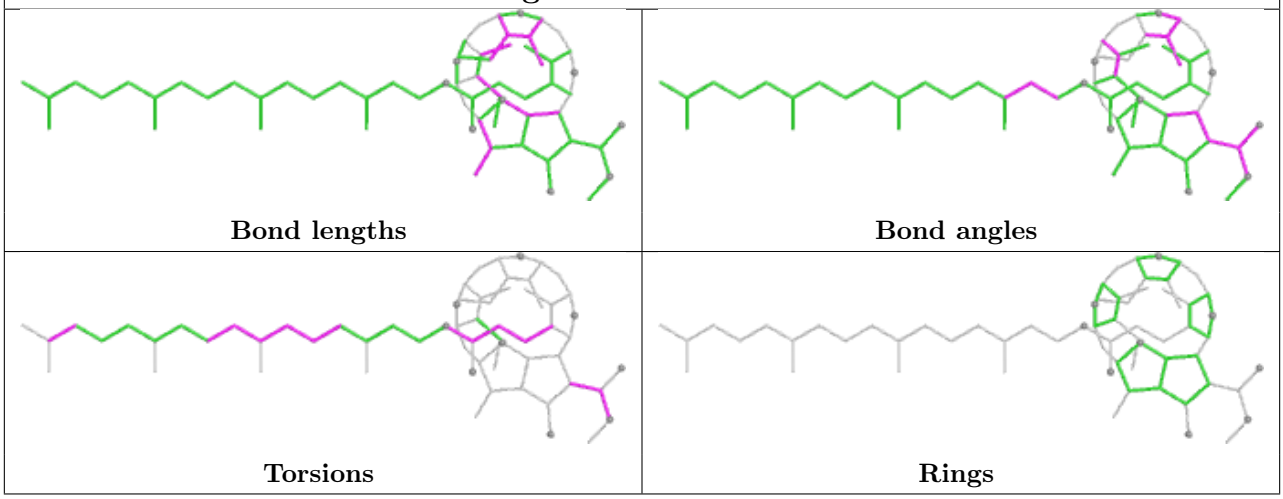


Rings

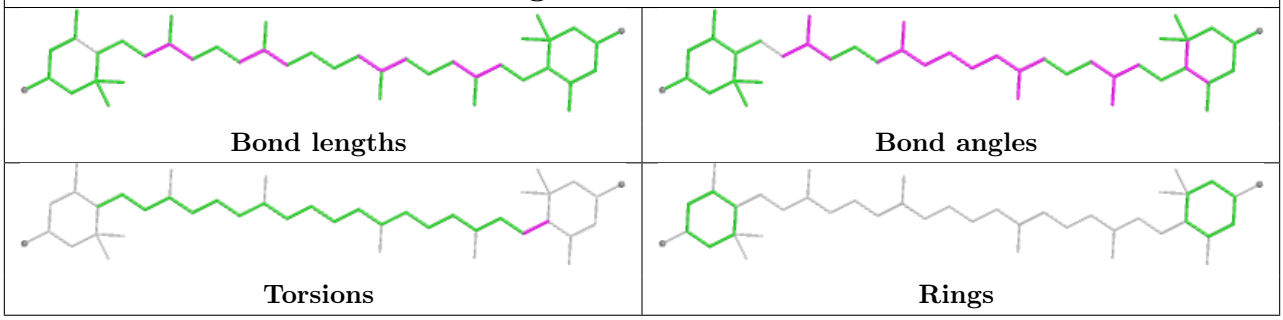
Ligand CHL 6 609

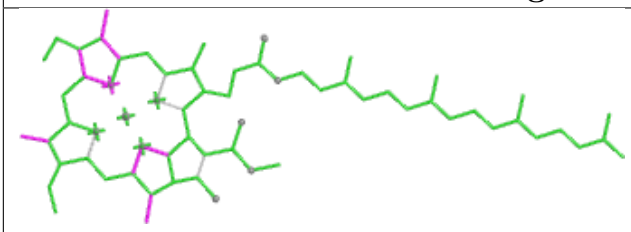
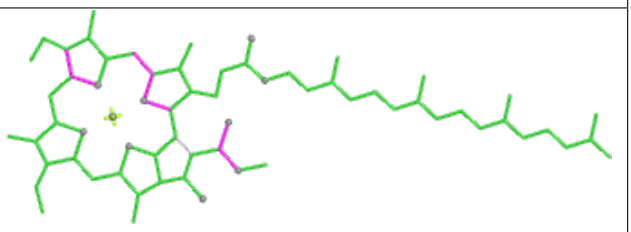
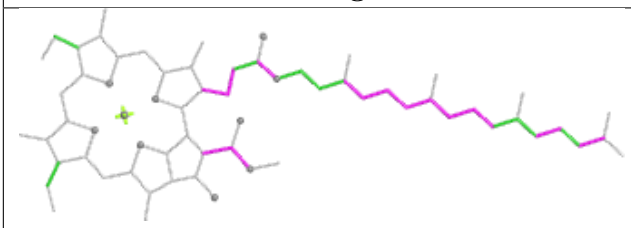
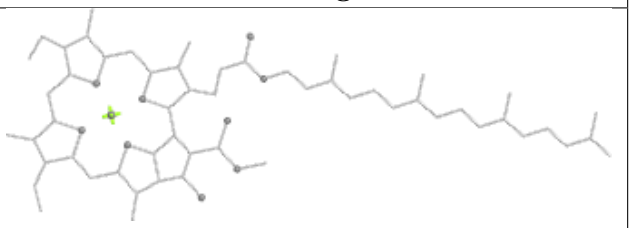


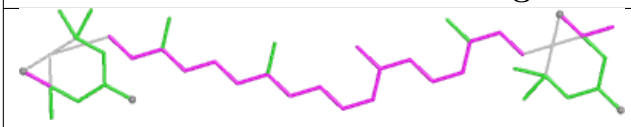
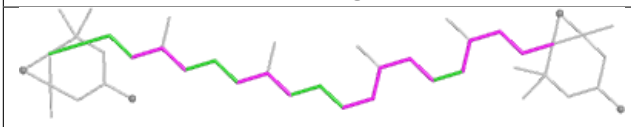
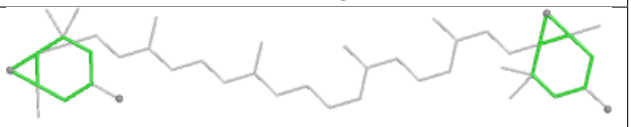
Ligand PHO R 408

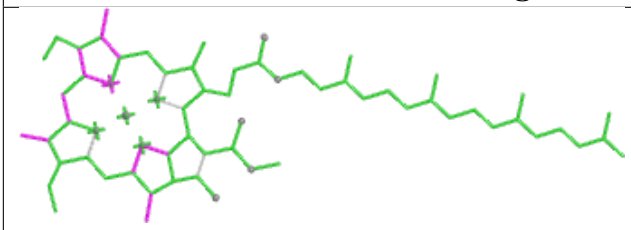
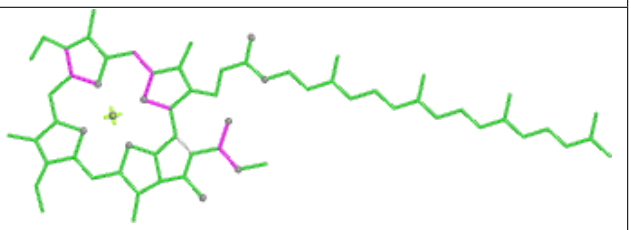
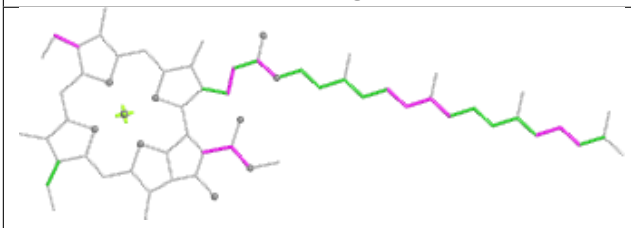
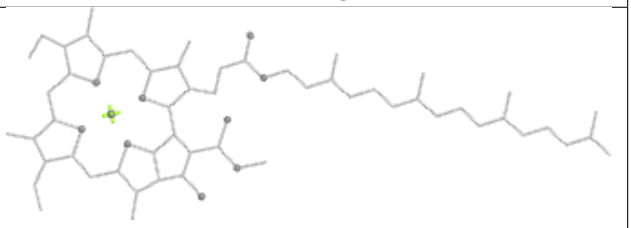


Ligand LUT n 616

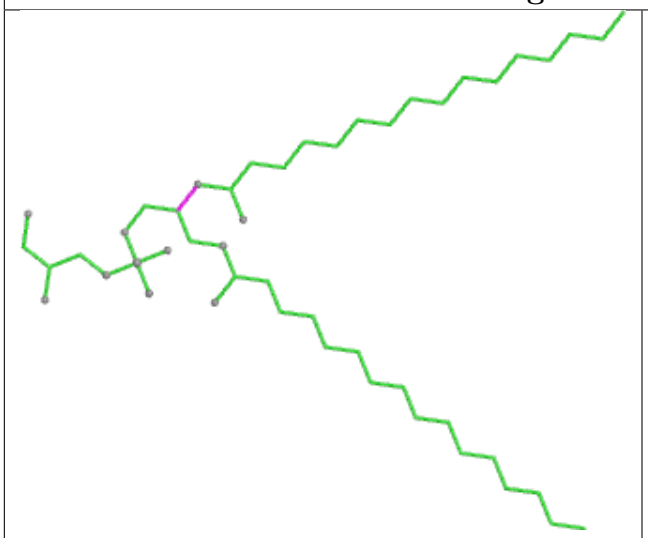


Ligand CLA v 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

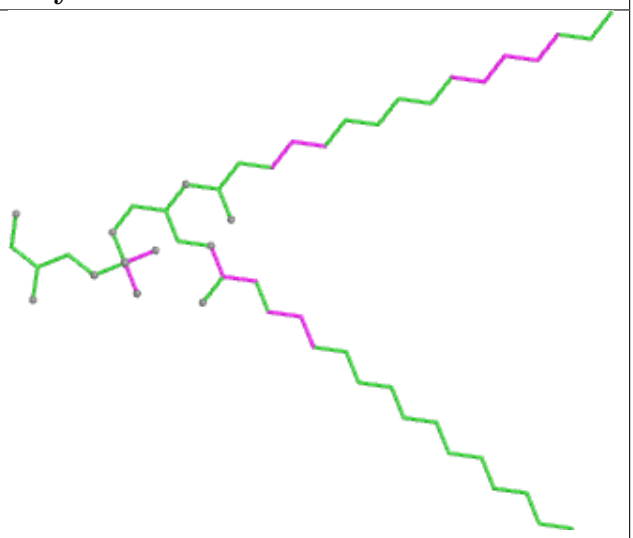
Ligand XAT Au 619	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA Au 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

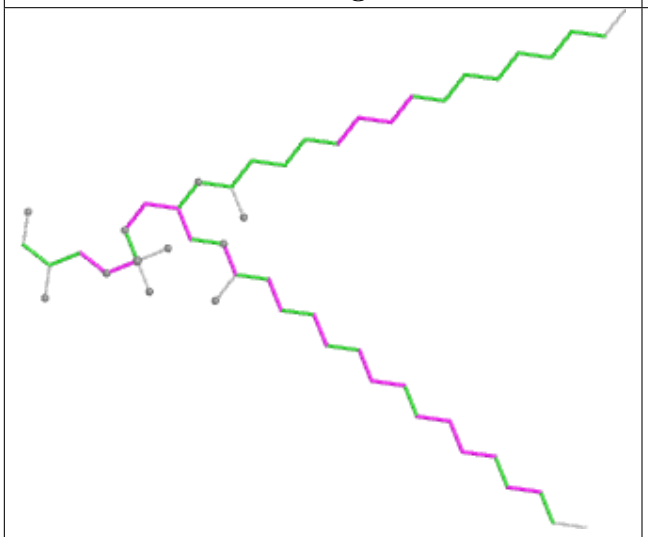
Ligand LHG y 319



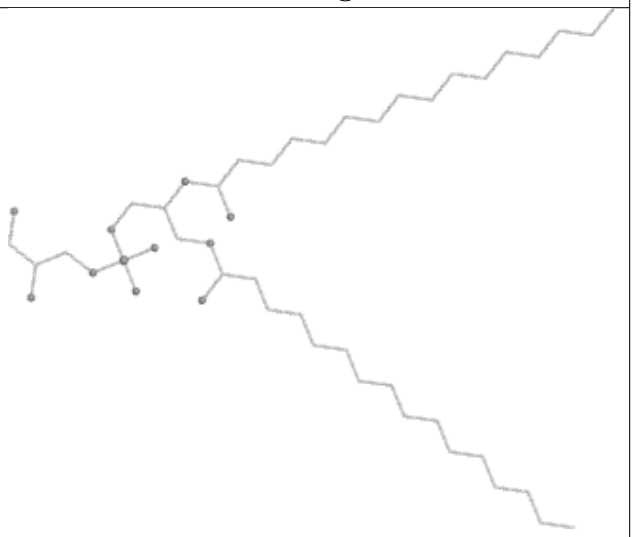
Bond lengths



Bond angles

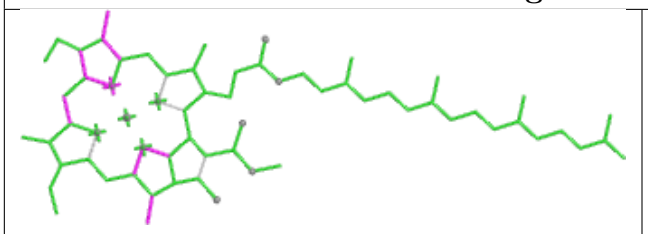


Torsions

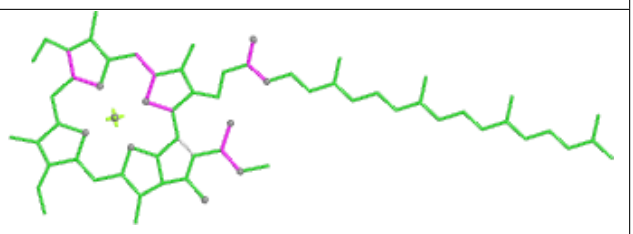


Rings

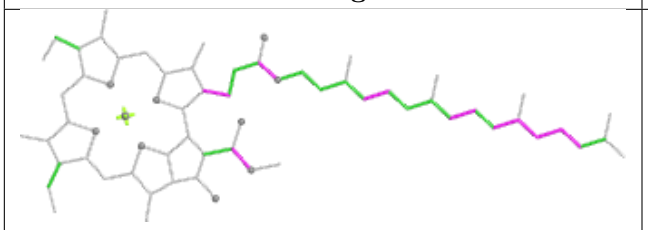
Ligand CLA C 513



Bond lengths



Bond angles



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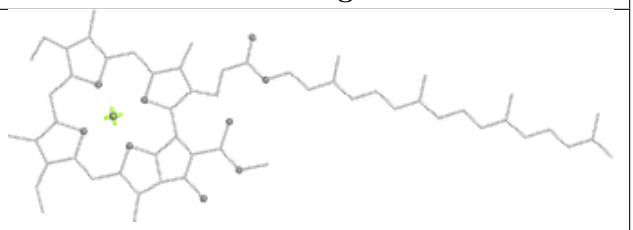
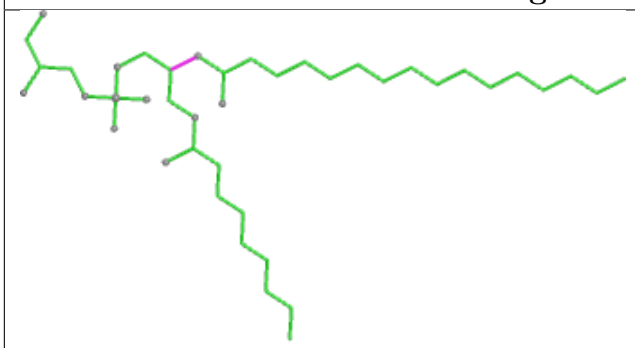
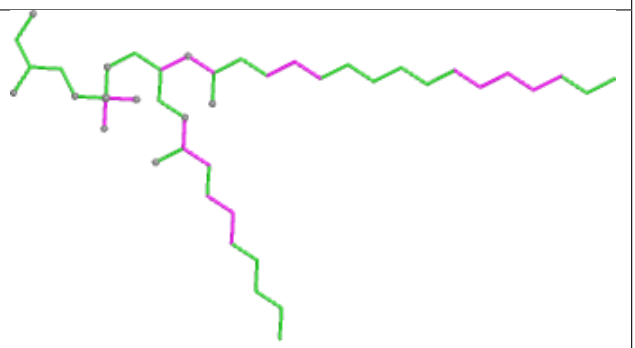
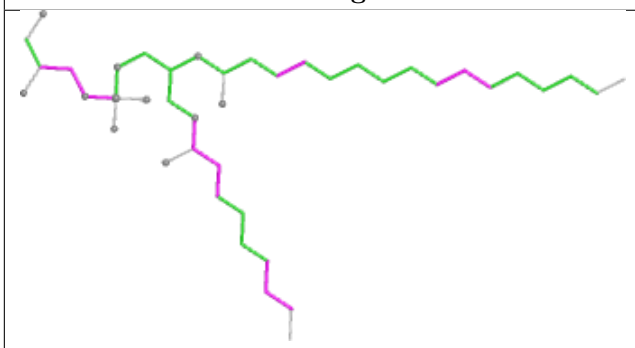
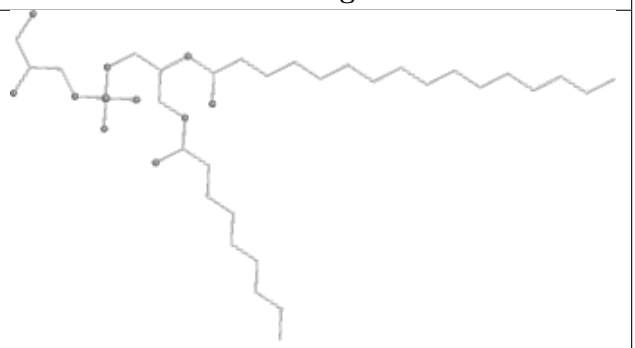
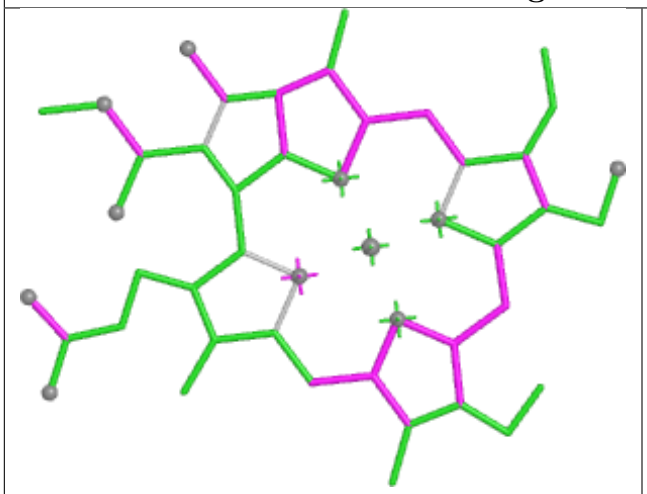


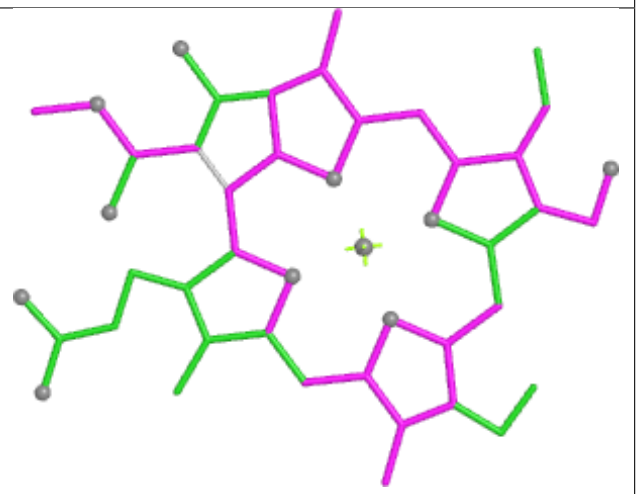
Rings

Ligand LHG r 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

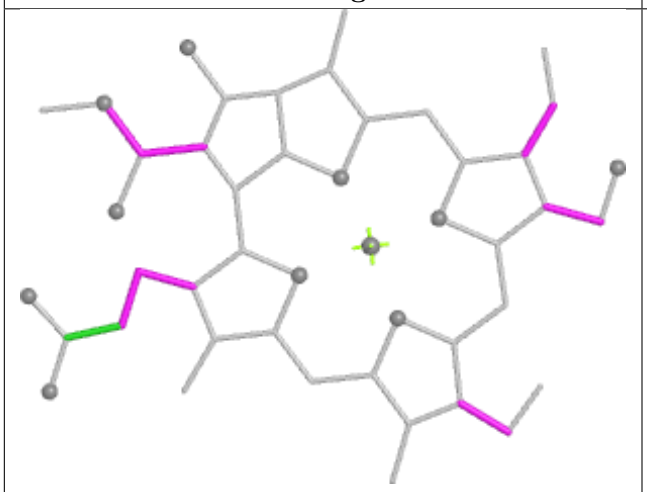
Ligand CHL S 607



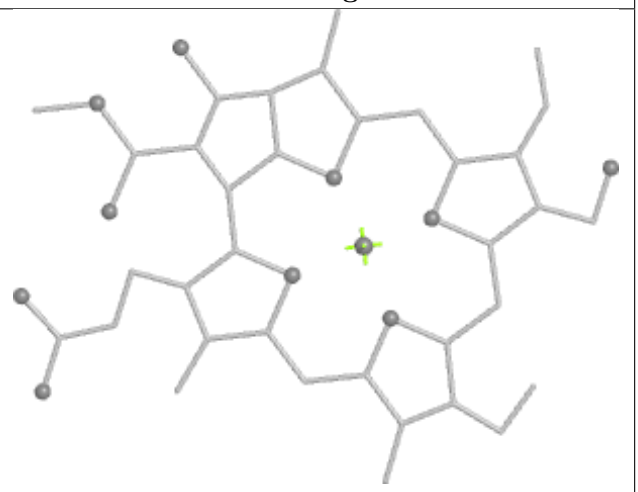
Bond lengths



Bond angles

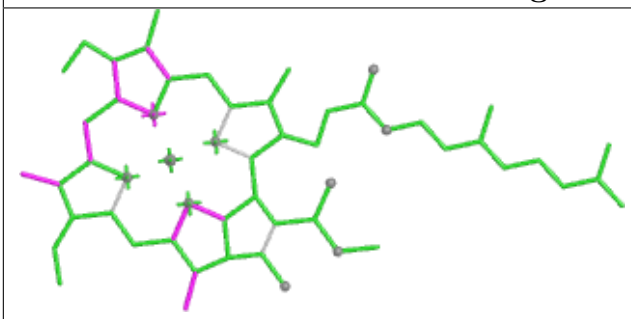


Torsions



Rings

Ligand CLA s 609



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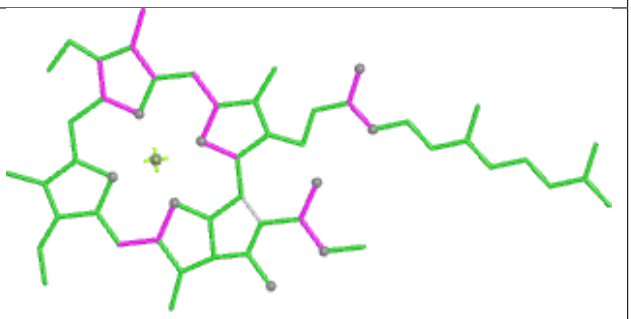
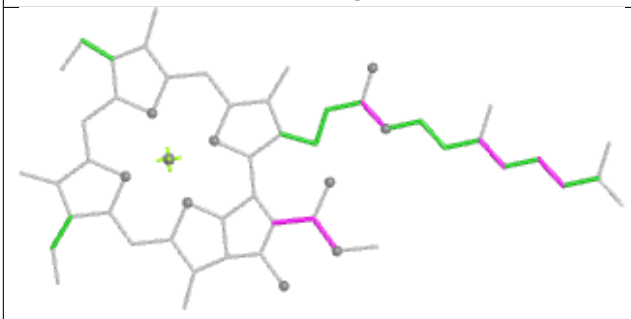


Bond angles



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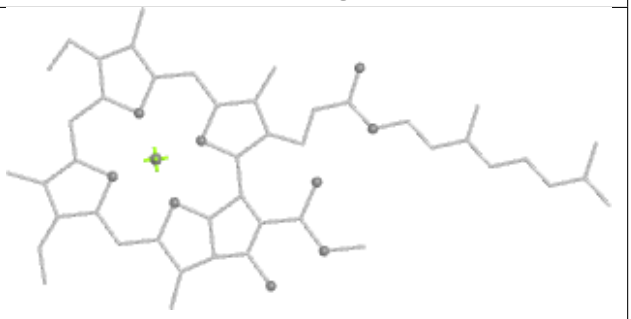
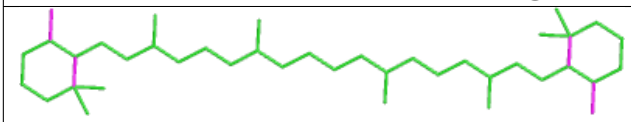


Rings

Ligand BCR 1 515



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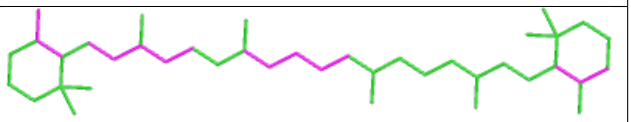
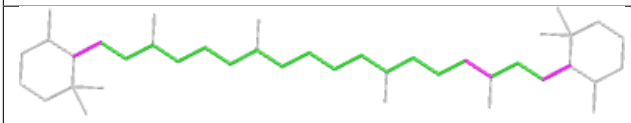
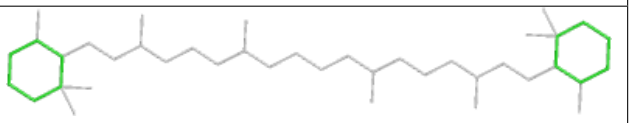


Bond angles

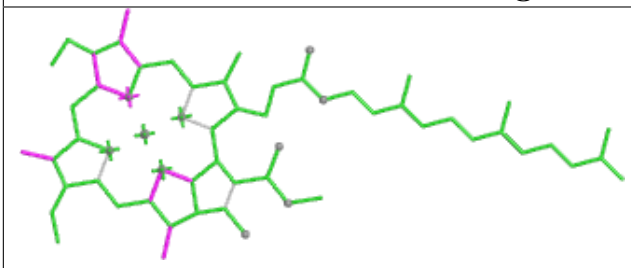


Torsions

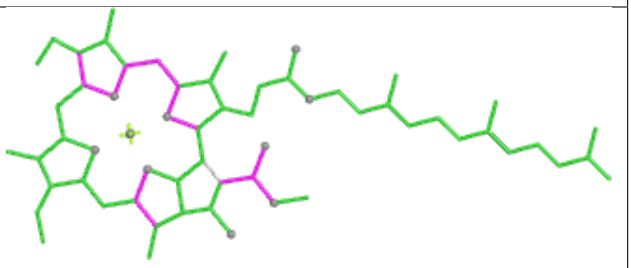


Rings

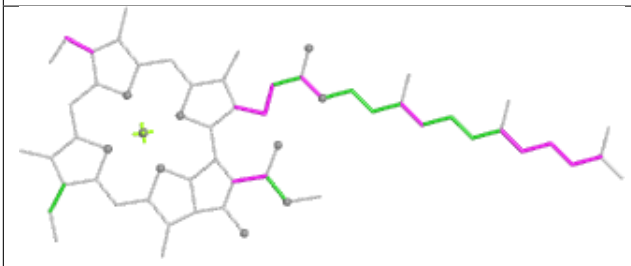
Ligand CLA A2 611



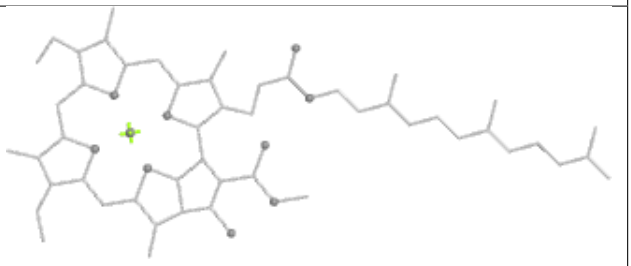
Bond lengths



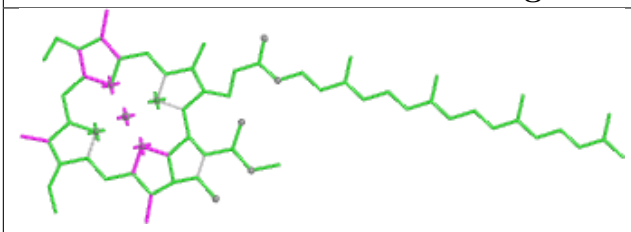
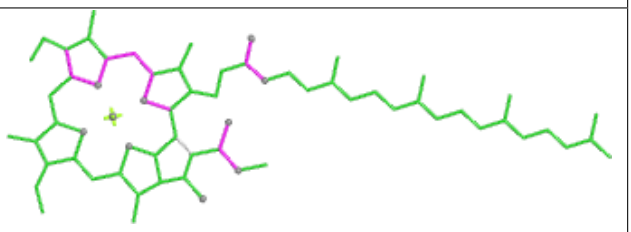
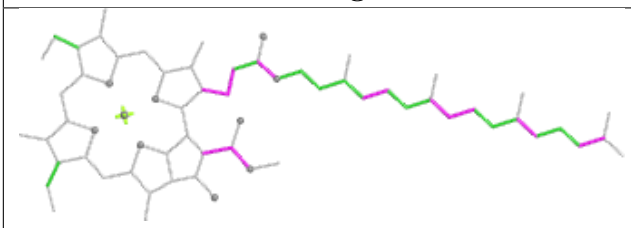
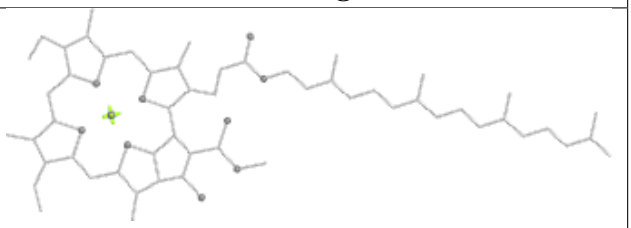
Bond angles



Torsions



Rings

Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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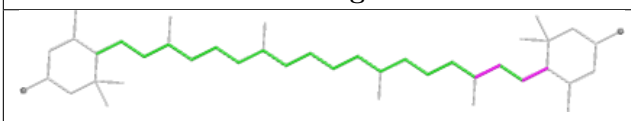
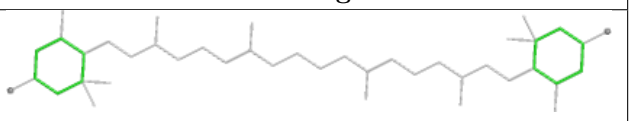
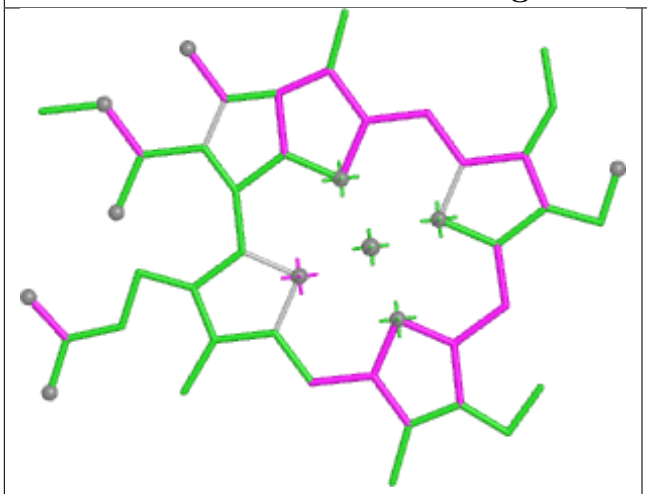
Bond lengths	Bond angles
 Torsions	 Rings

Ligand CHL AB 304



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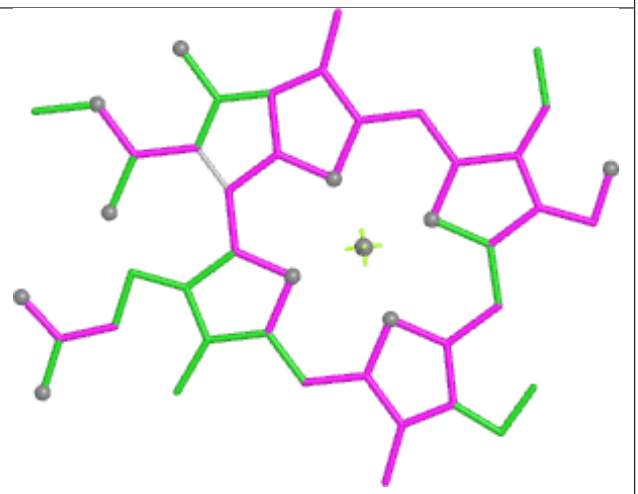

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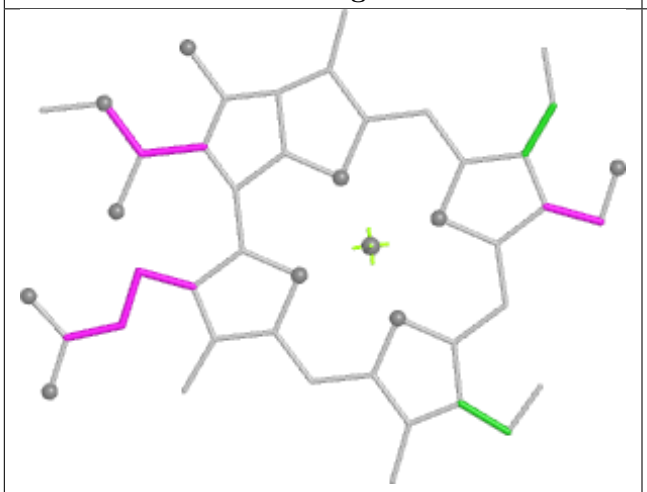

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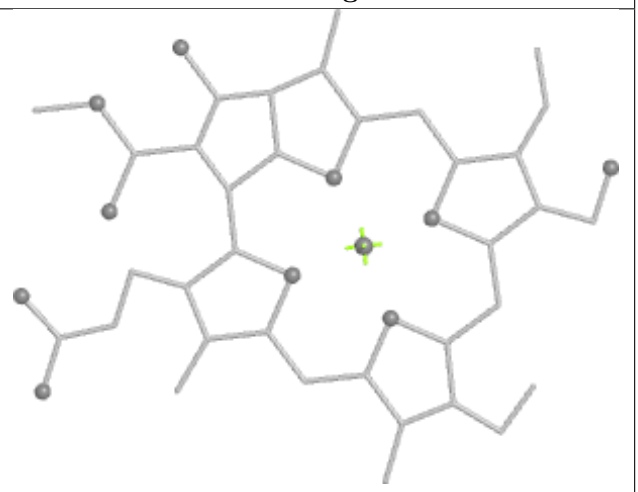
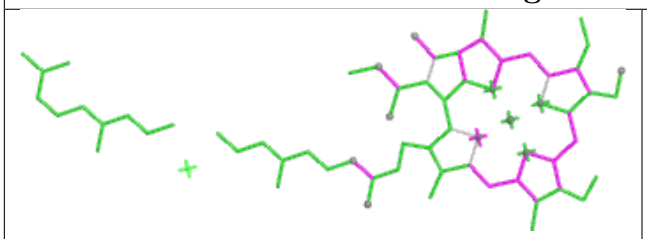


Rings

Ligand CHL G 601



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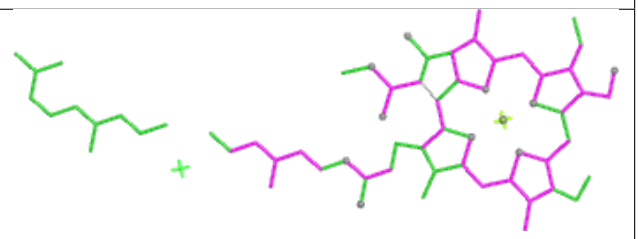

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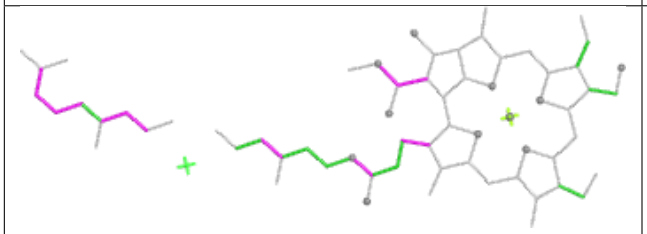

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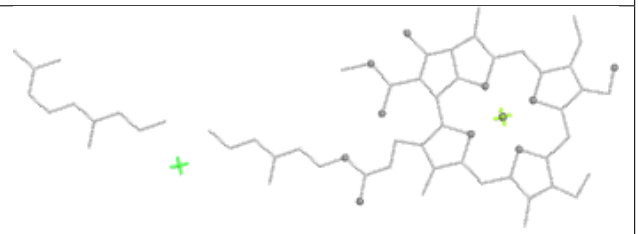

Rings

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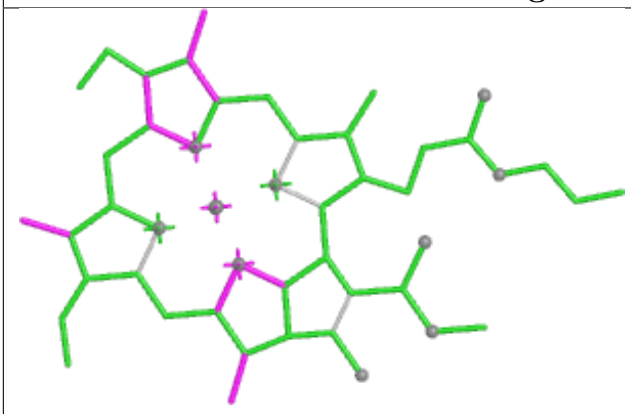
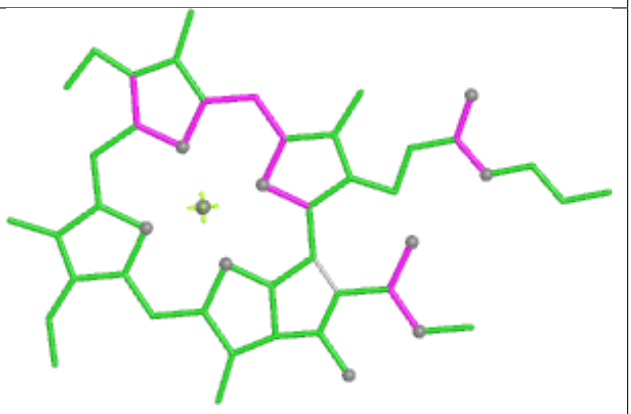
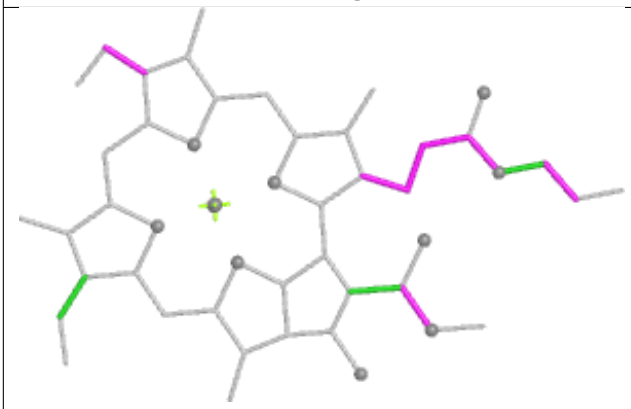
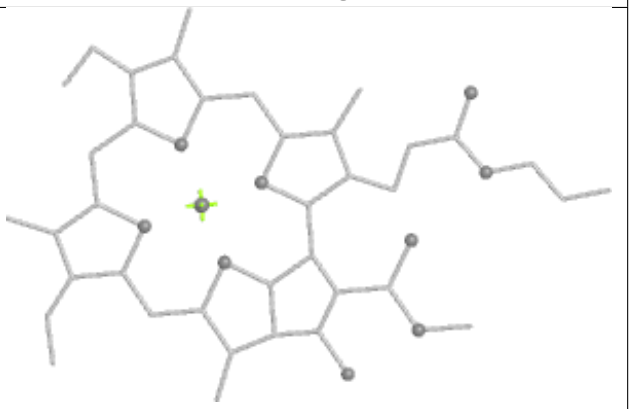
 Bond lengths	 Bond angles
 Torsions	 Rings

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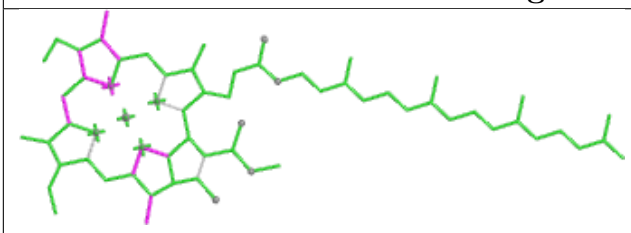
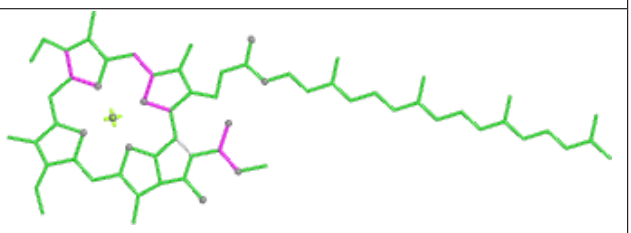
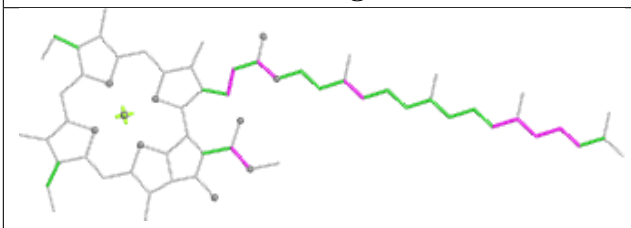
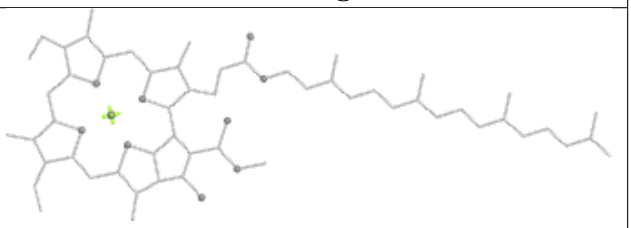
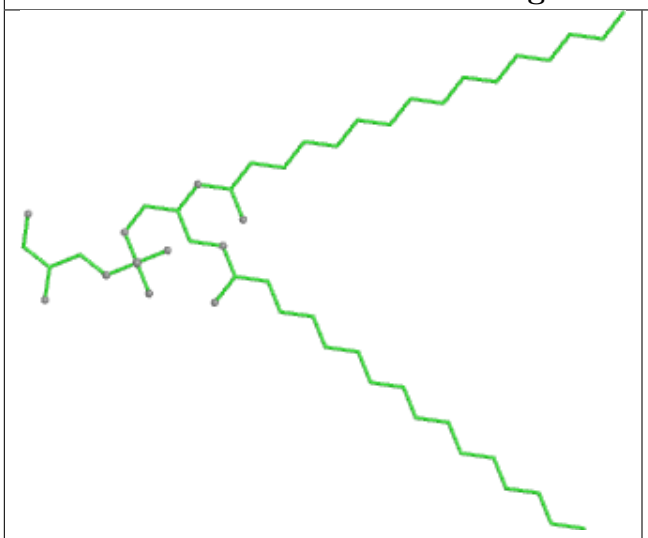
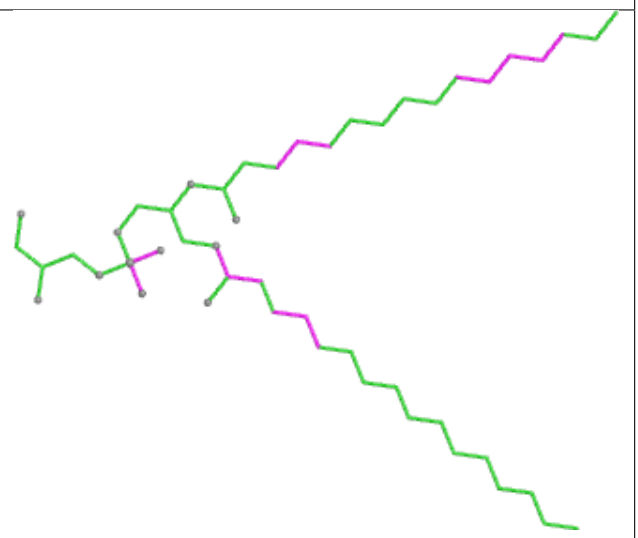
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 1 521



Bond lengths



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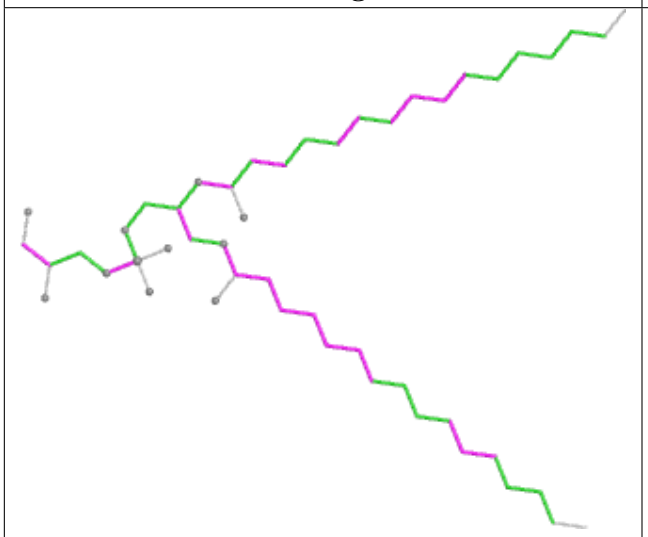

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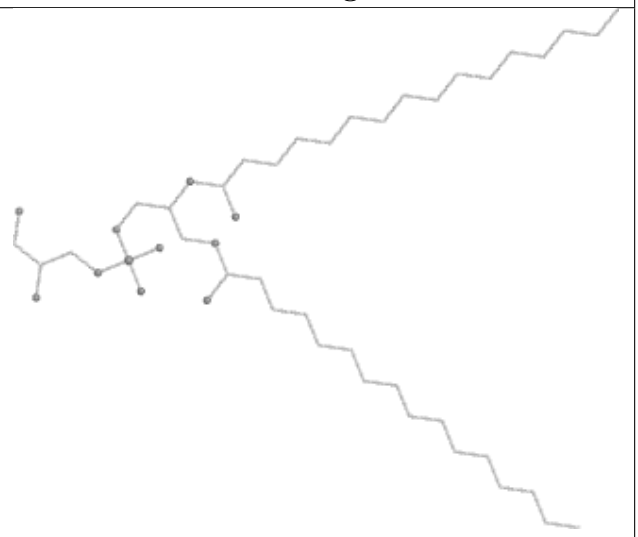
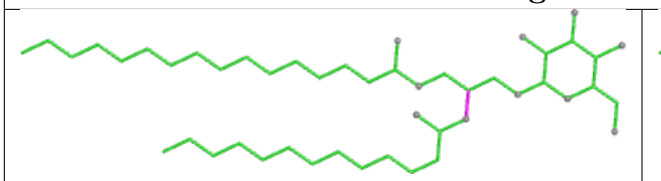


Rings

Ligand LMG i 101



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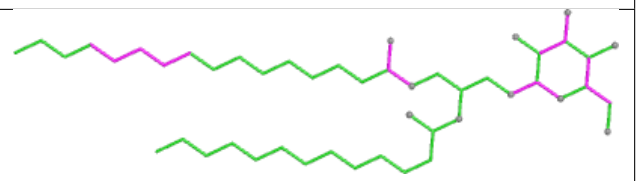

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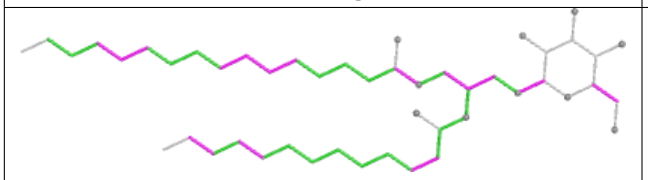

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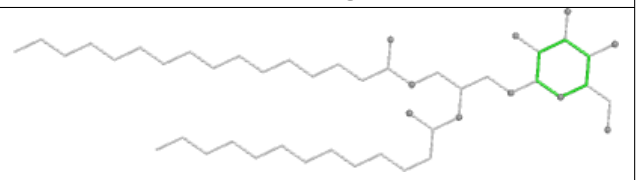
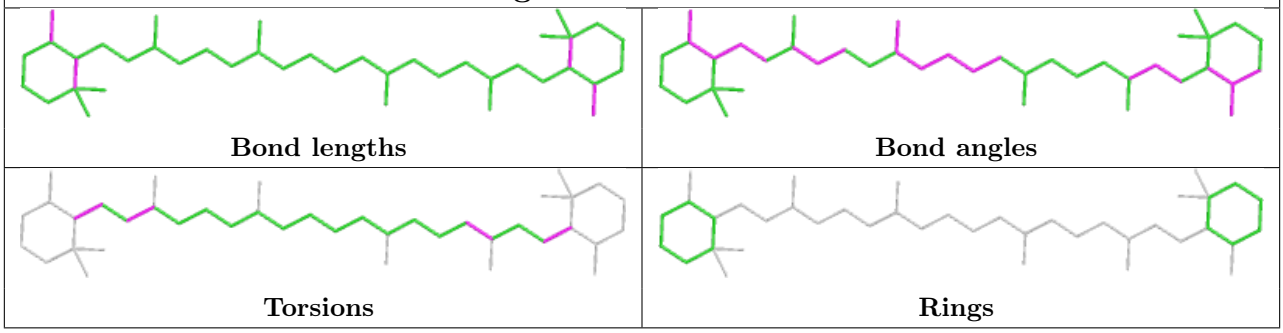
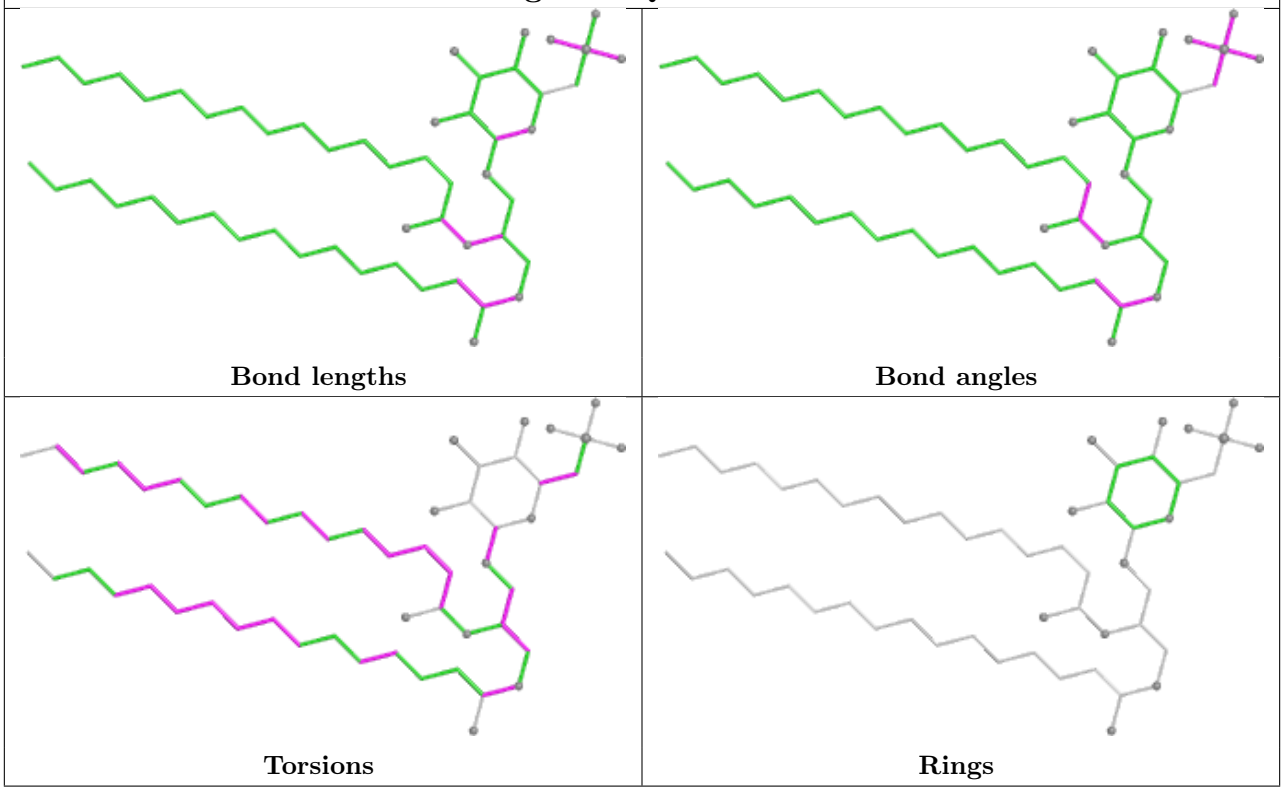


Rings

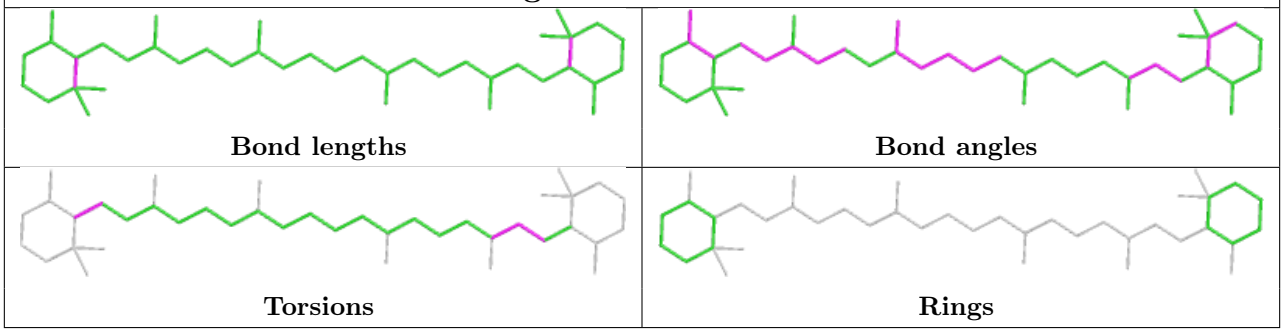
Ligand BCR Bb 101



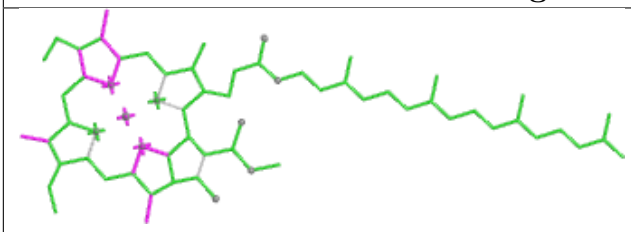
Ligand SQD A 413



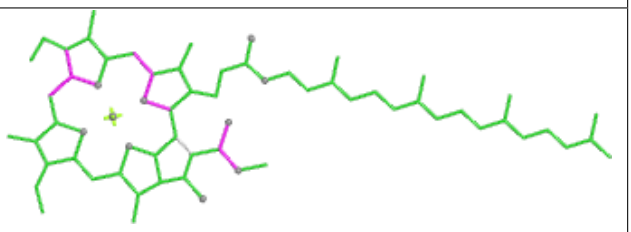
Ligand BCR B 617



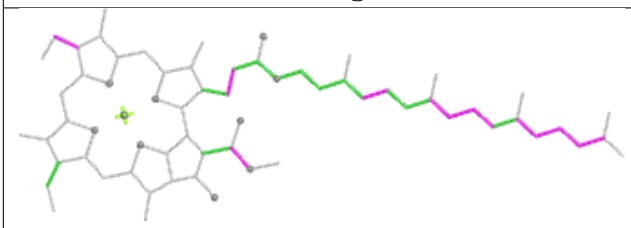
Ligand CLA c 508



Bond lengths



Bond angles



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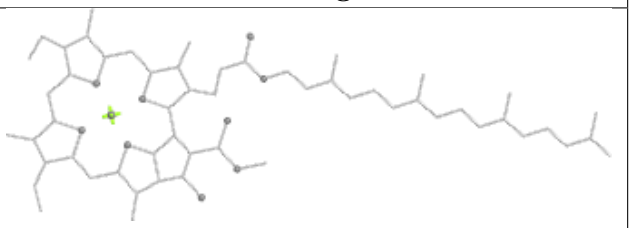
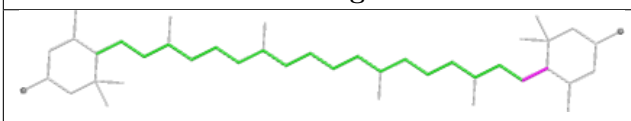


Rings

Ligand LUT 8 311

Bond lengths

Bond angles



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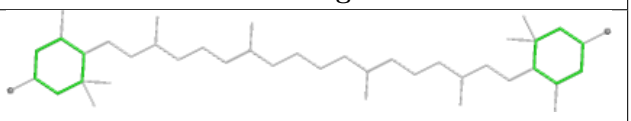

Rings

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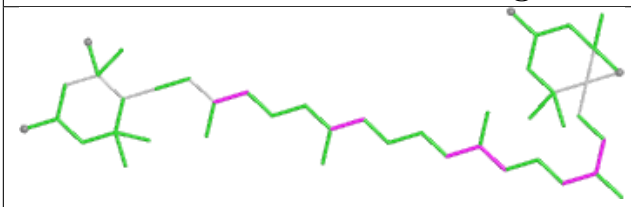

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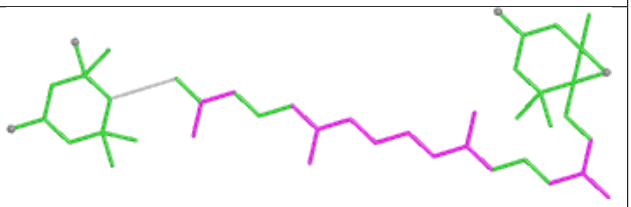
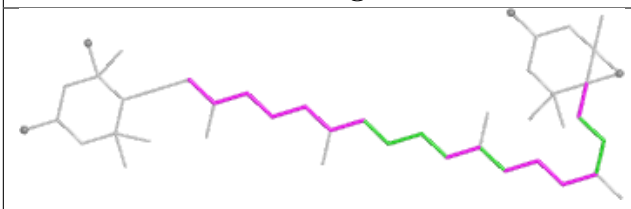


Bond angles



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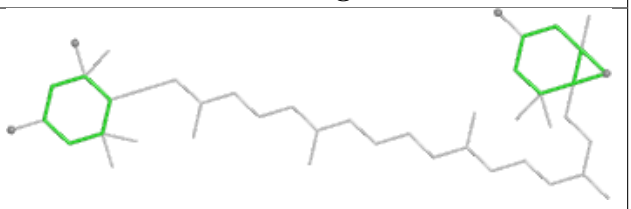
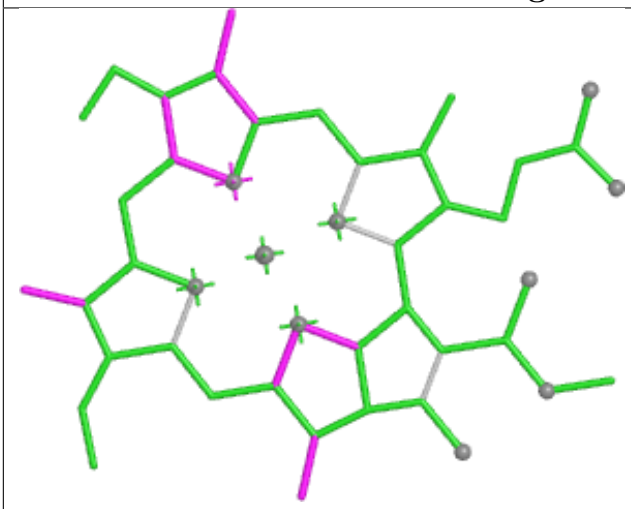


Rings

Ligand CLA 0 604



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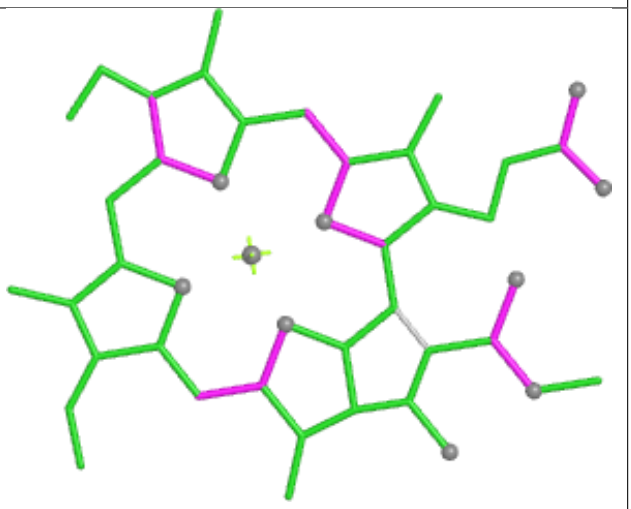
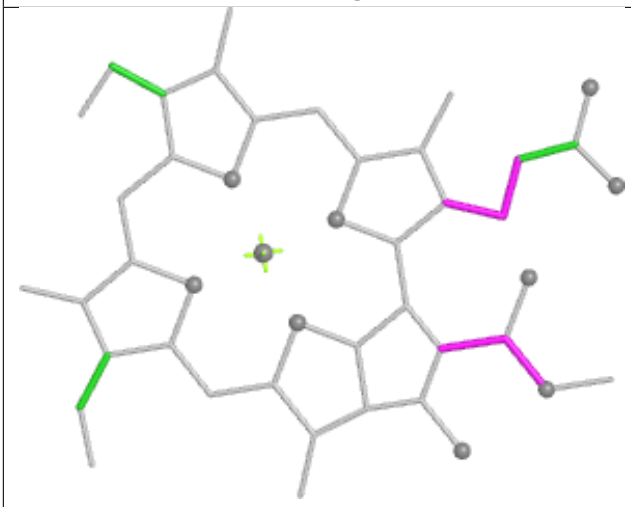


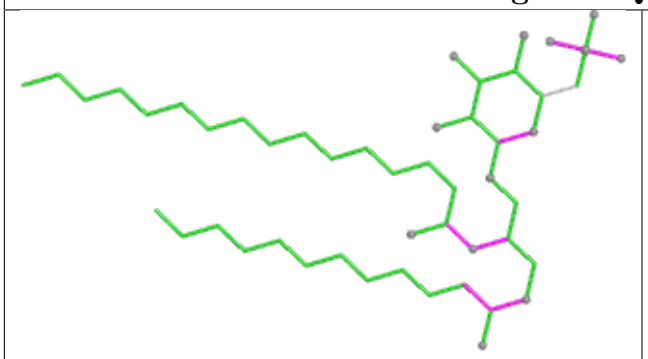
Bond angles



Torsions

Rings

Ligand SQD BG 406



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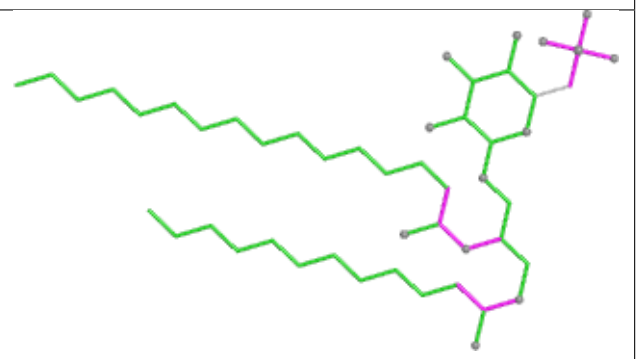

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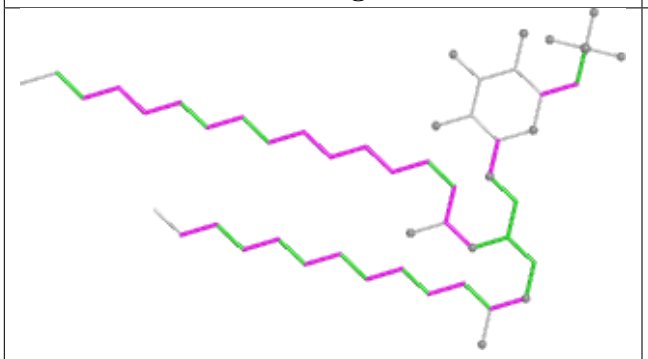

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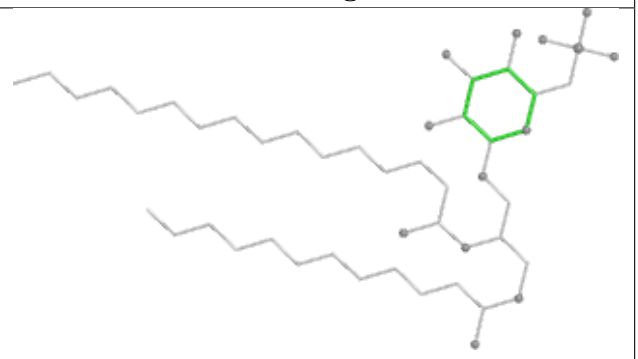
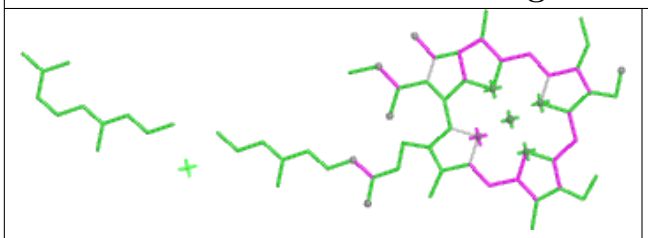


Rings

Ligand CHL n 607



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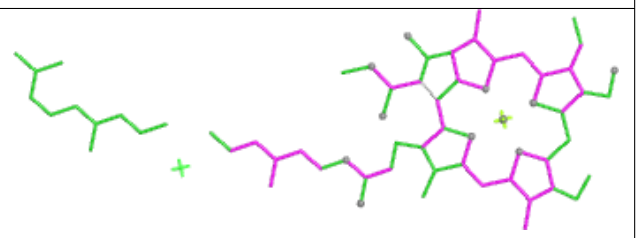
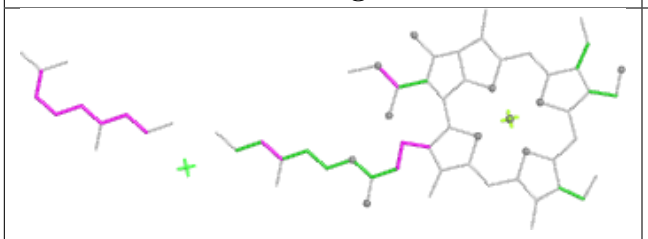


Bond angles



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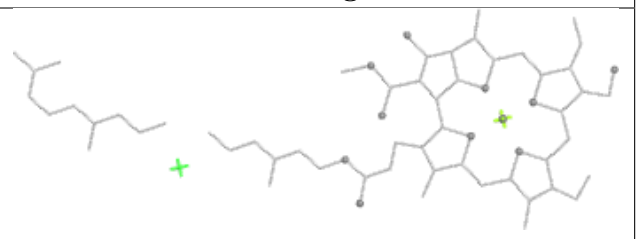
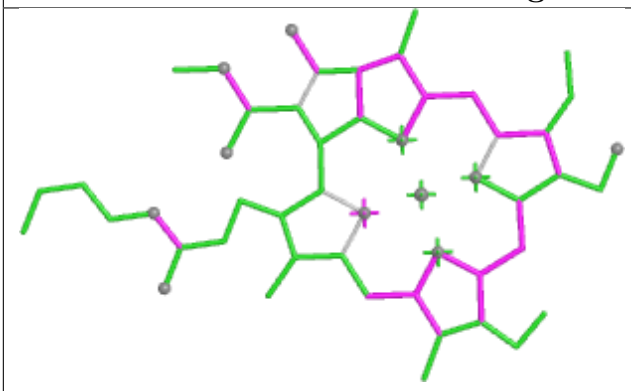
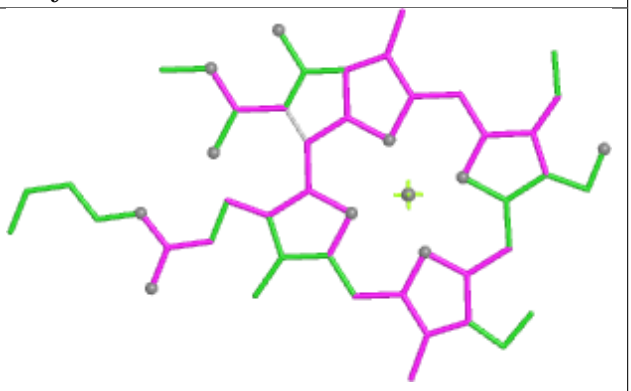
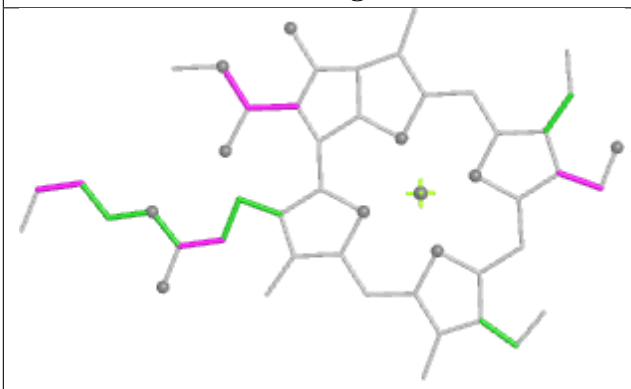
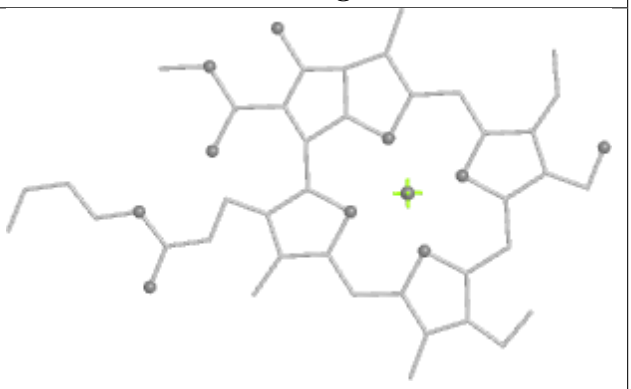
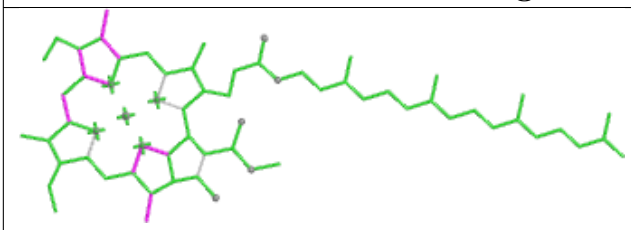
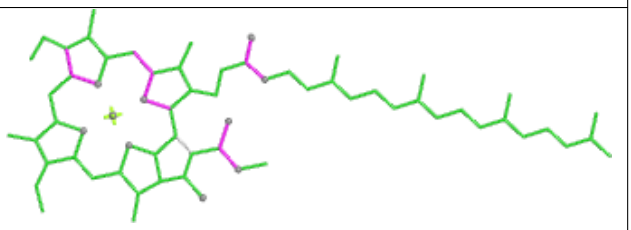
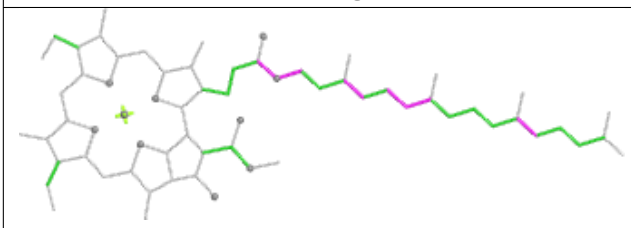
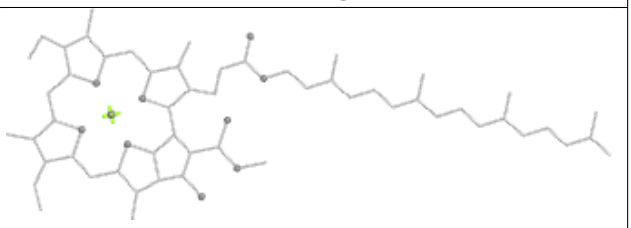
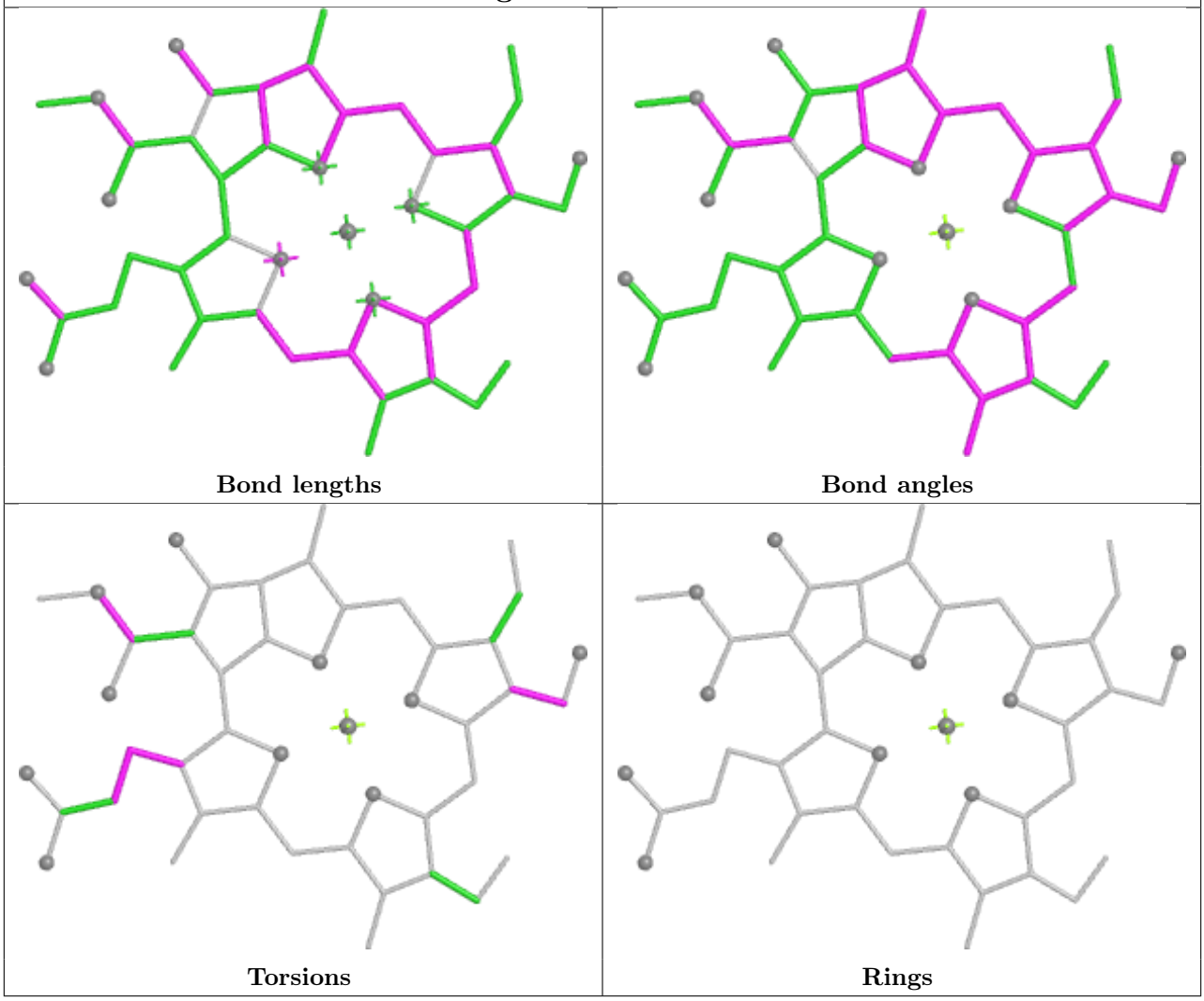


Rings

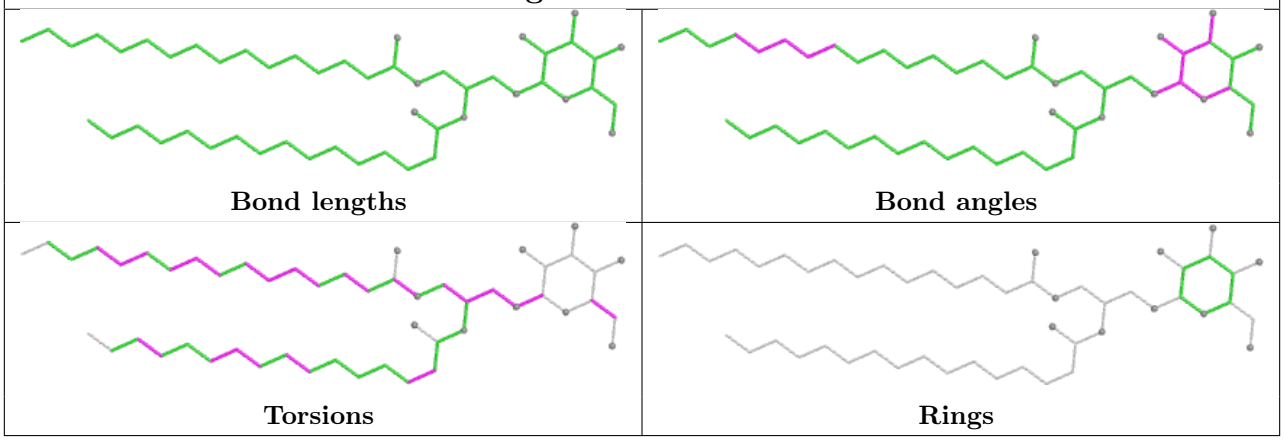
Ligand CHL y 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Ba 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

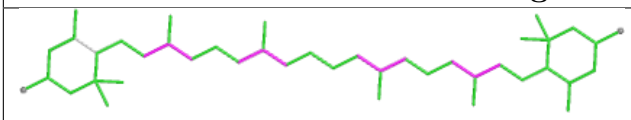
Ligand CHL 5 608



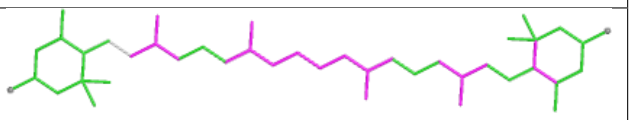
Ligand LMG c 501



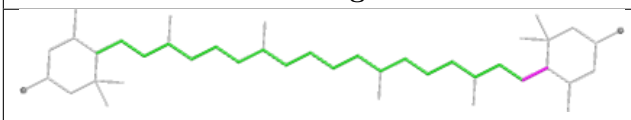
Ligand LUT s 615



Bond lengths



Bond angles



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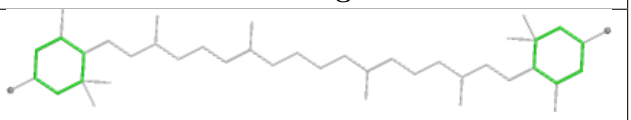
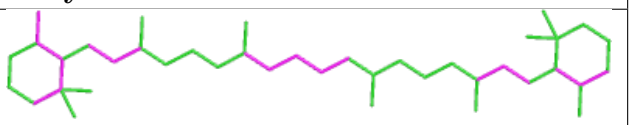


Rings

Ligand BCR Ay 101

Bond lengths



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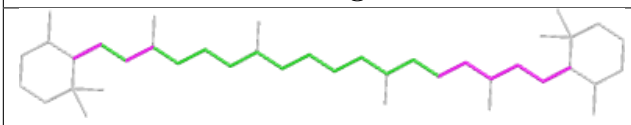

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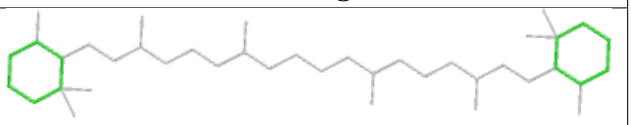
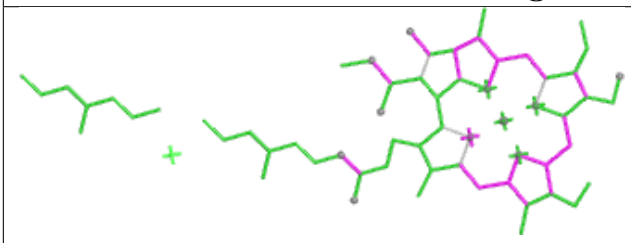


Rings

Ligand CHL 9 607



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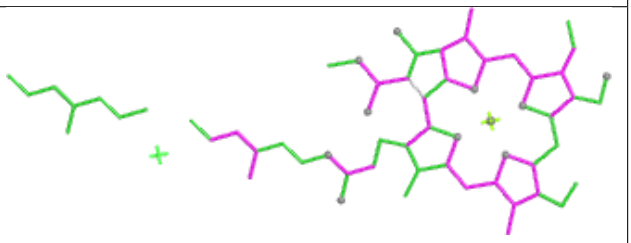

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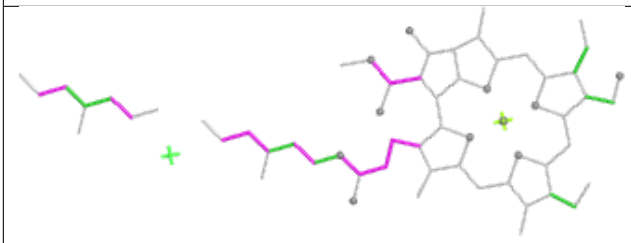

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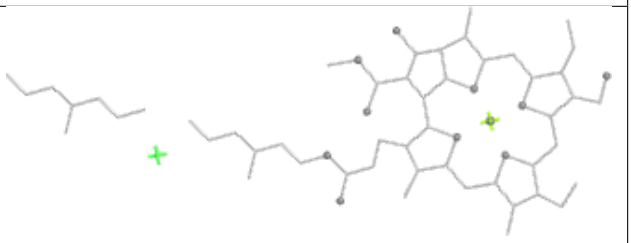
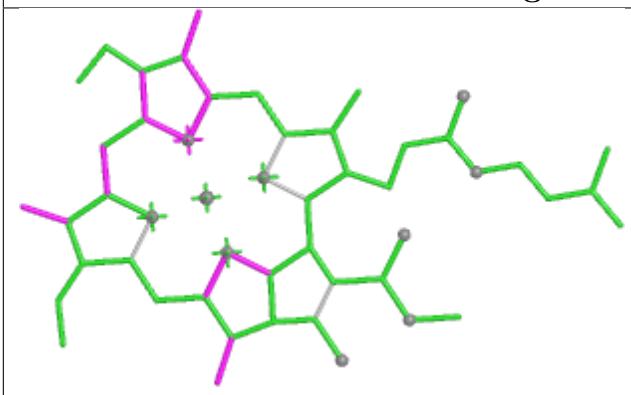
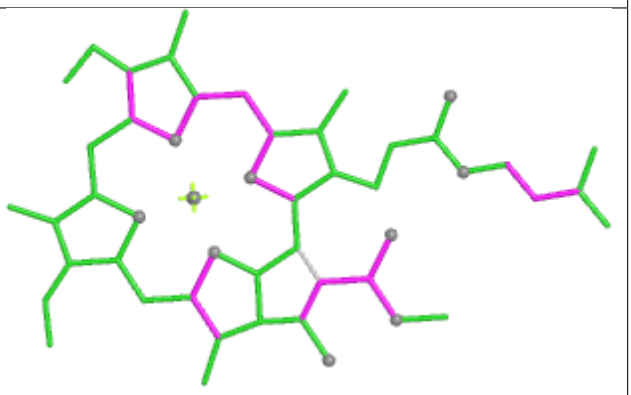
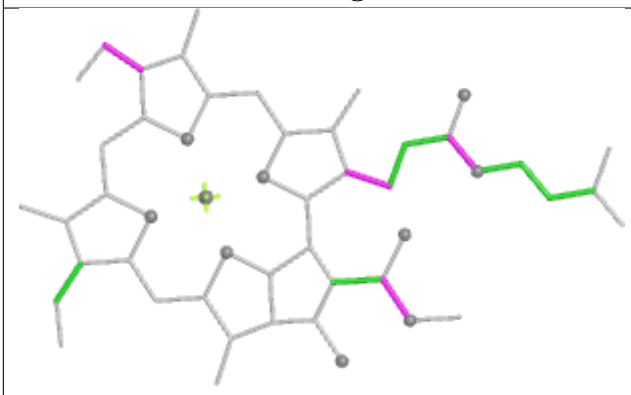
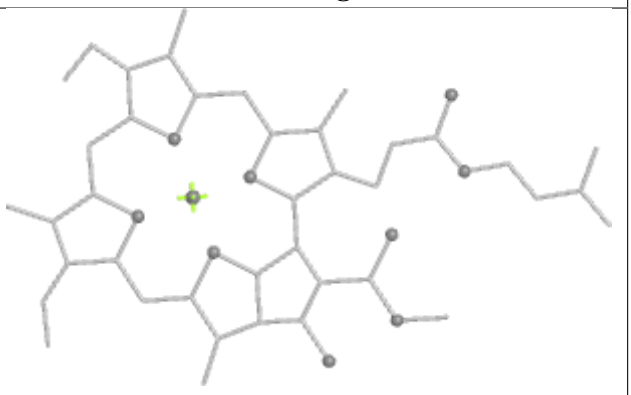


Rings

Ligand CLA A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

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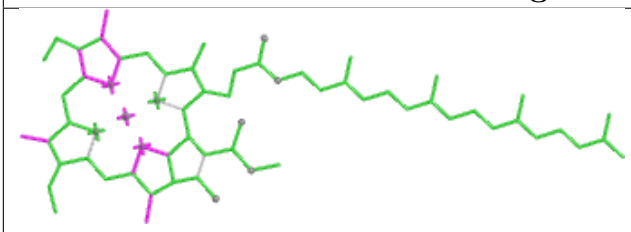
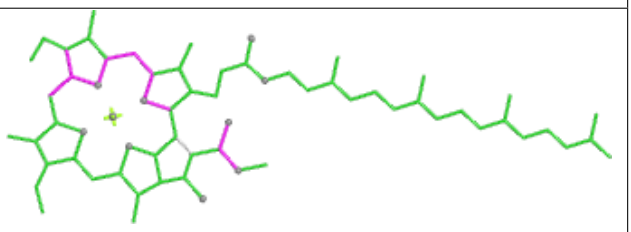
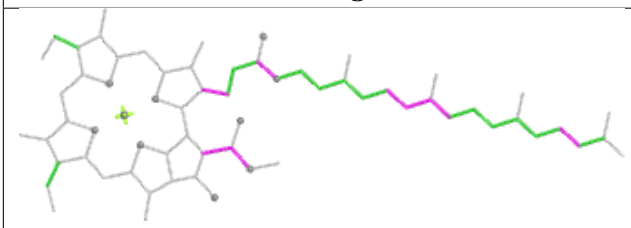
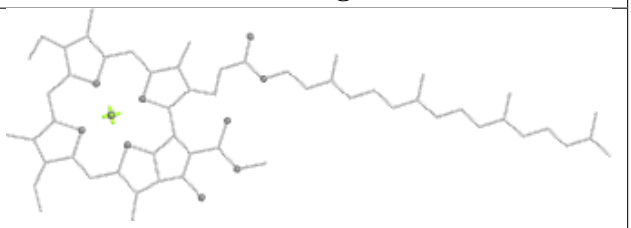
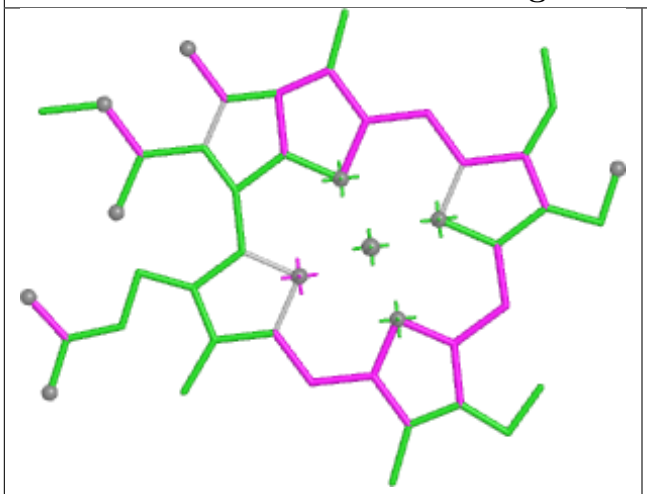
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 9 608



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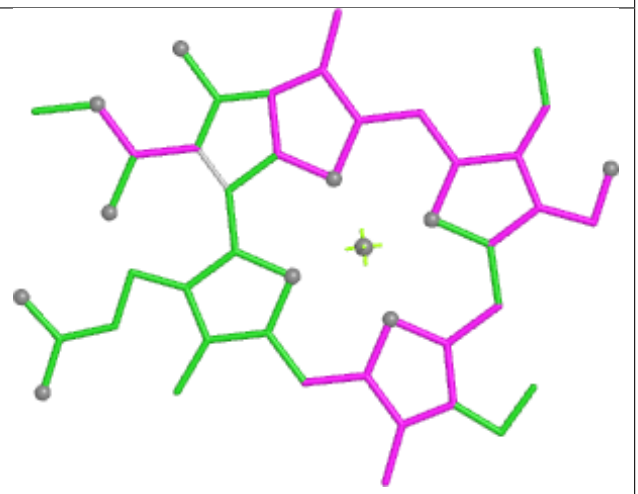
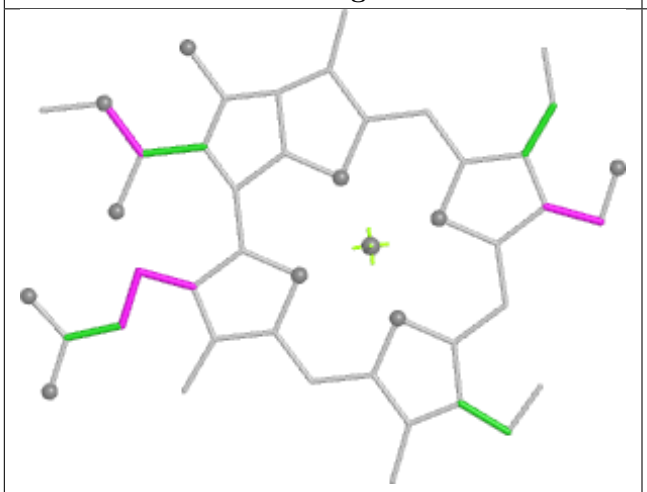


Bond angles



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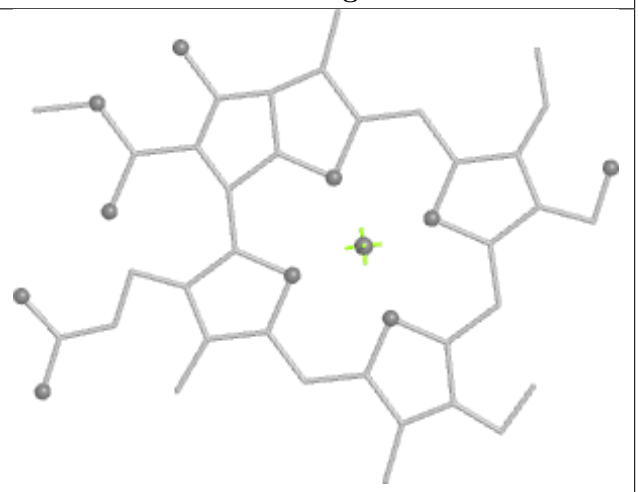
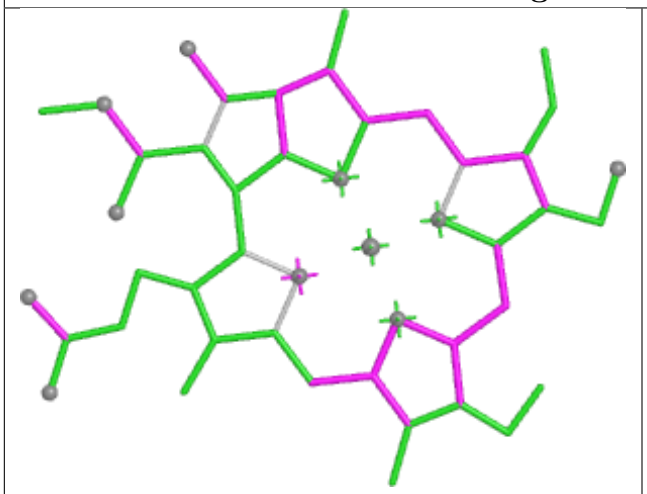


Rings

Ligand CHL s 607



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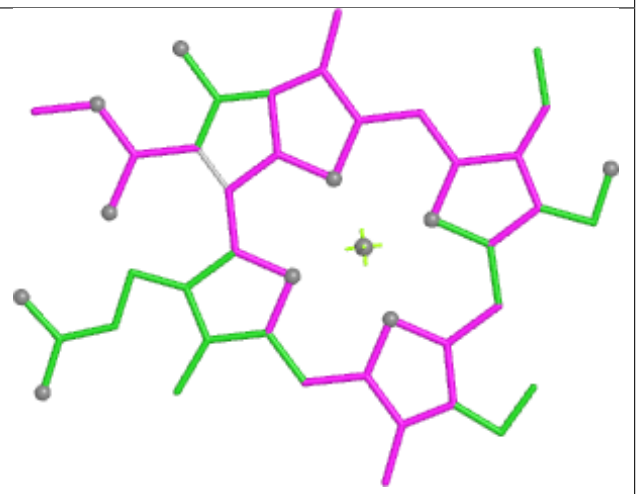

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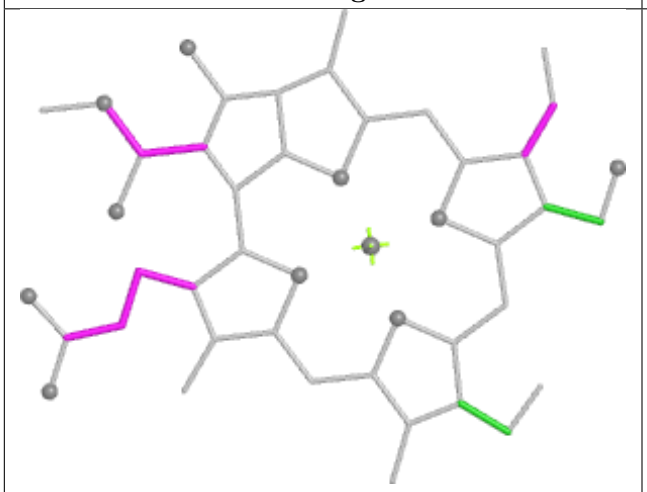

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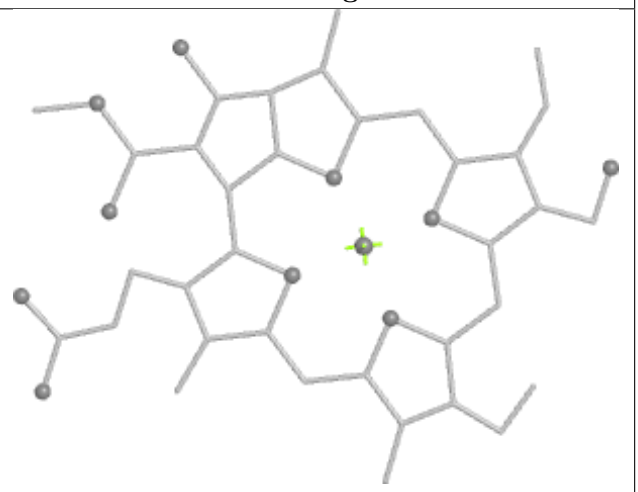
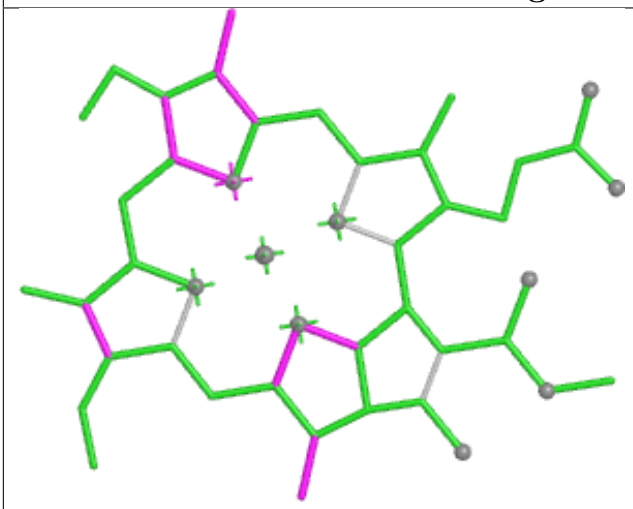


Rings

Ligand CLA 6 604



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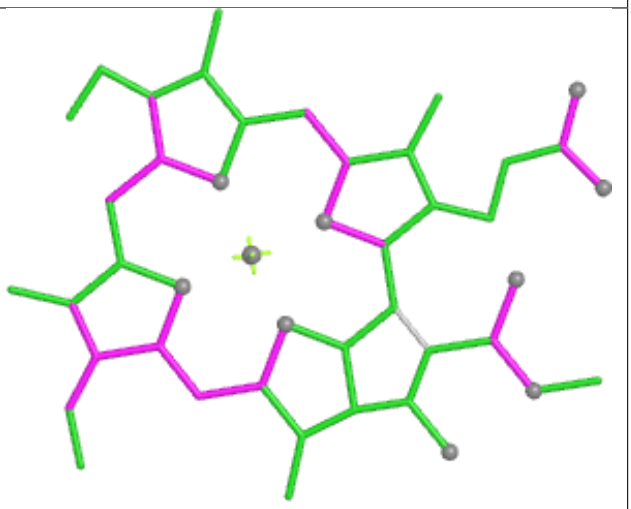

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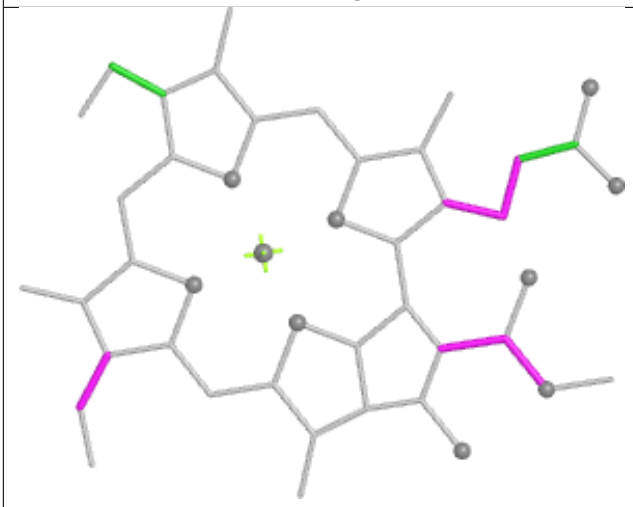
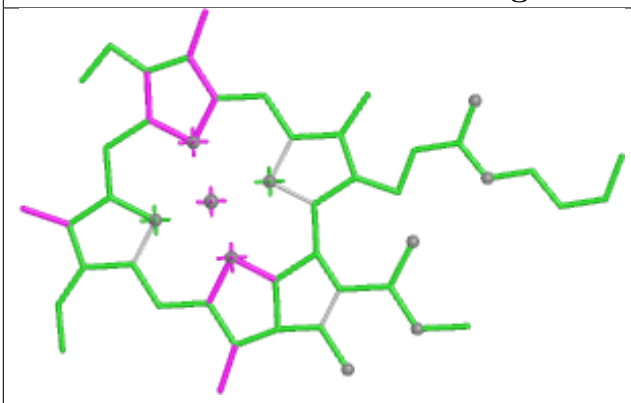
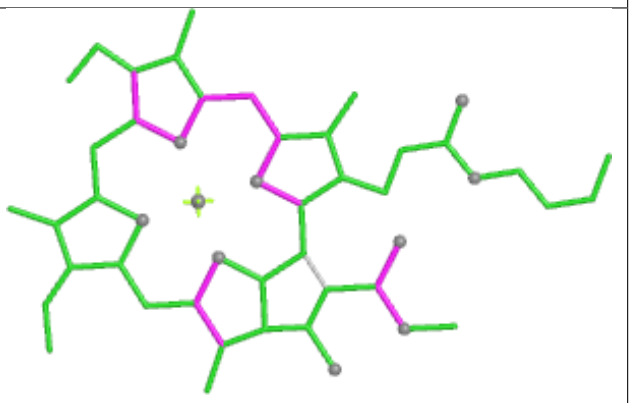
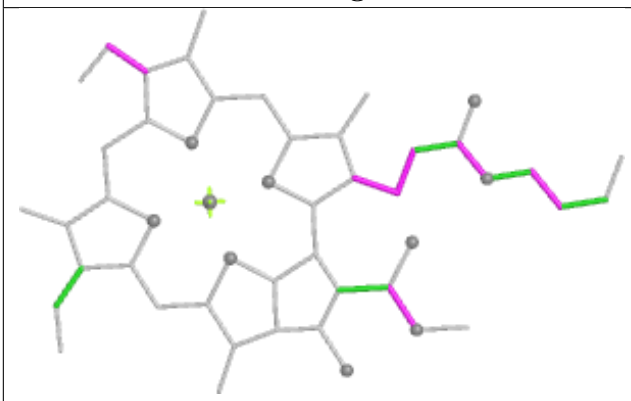
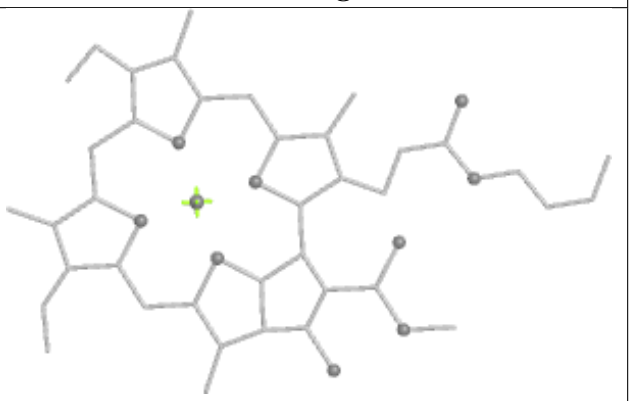


Torsions

Rings

Ligand CLA BU 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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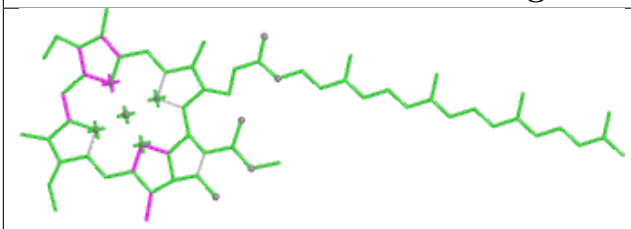
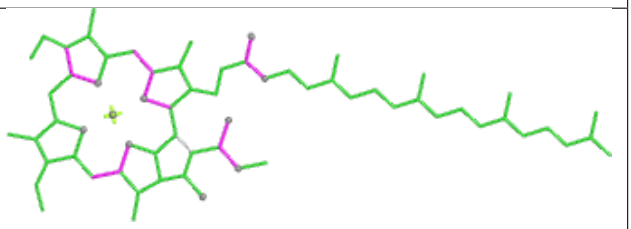
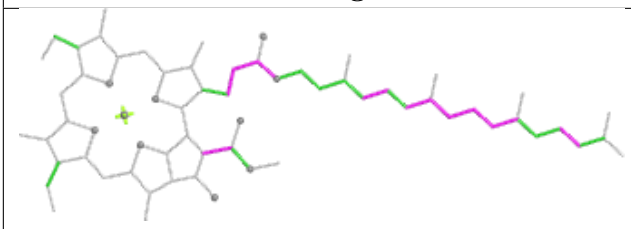
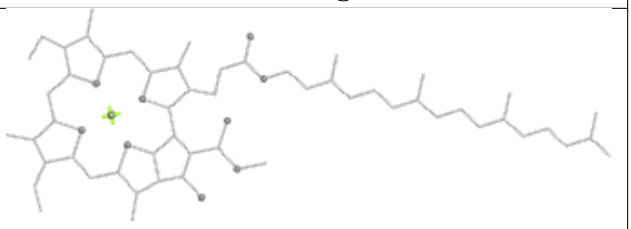
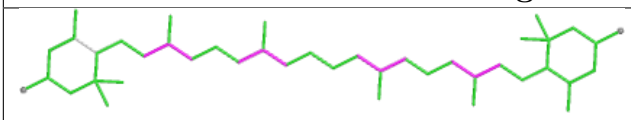
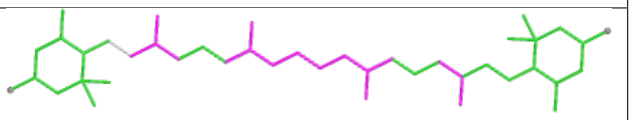
 Bond lengths	 Bond angles
 Torsions	 Rings

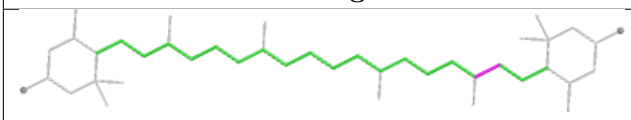
Ligand LUT Ba 316



Bond lengths



Bond angles



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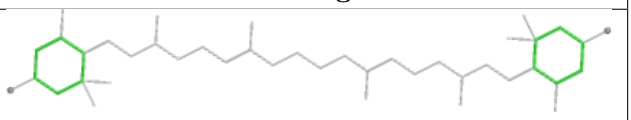
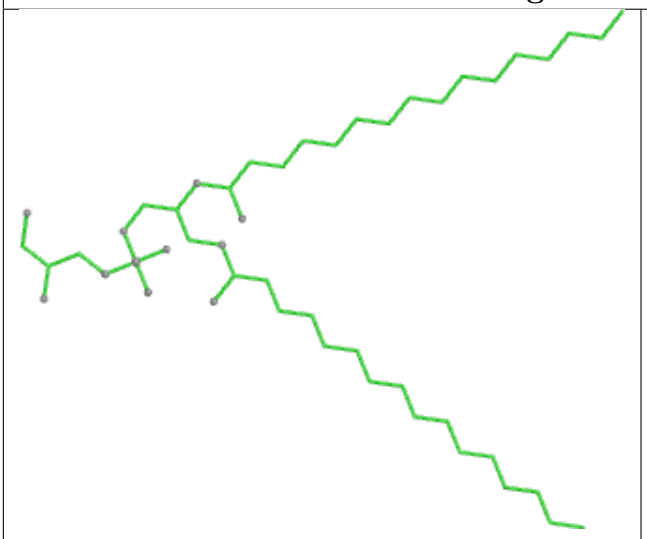
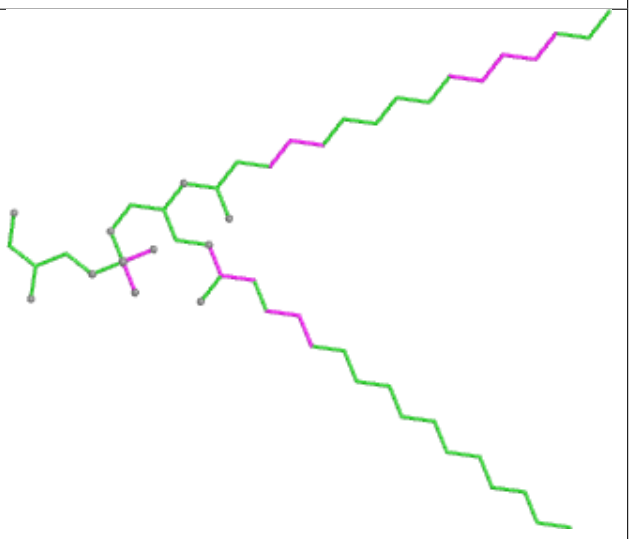


Rings

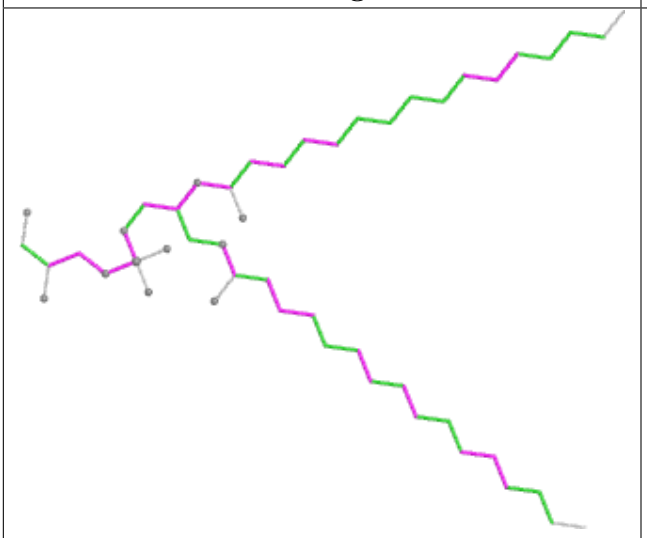
Ligand LHG 1 520



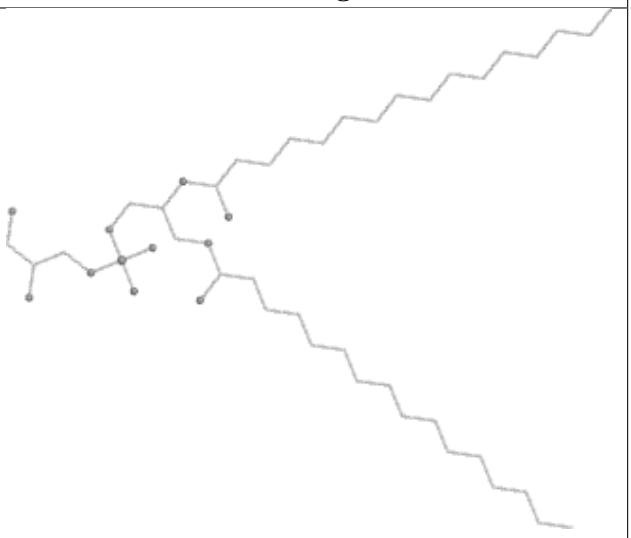
Bond lengths



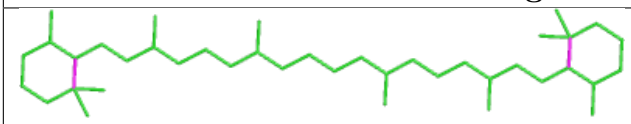
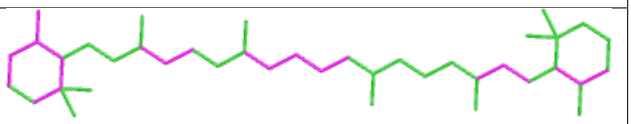
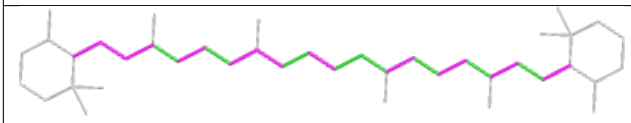
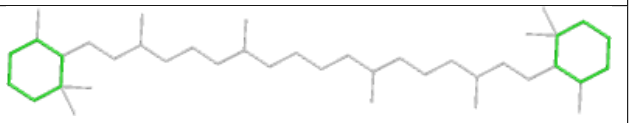
Bond angles



Torsions



Rings

Ligand BCR b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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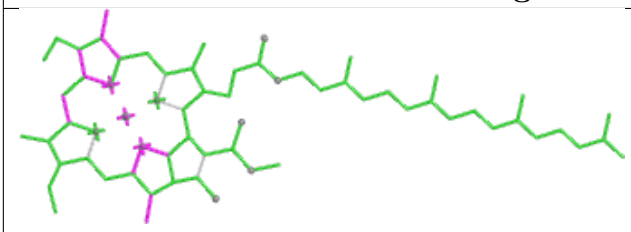
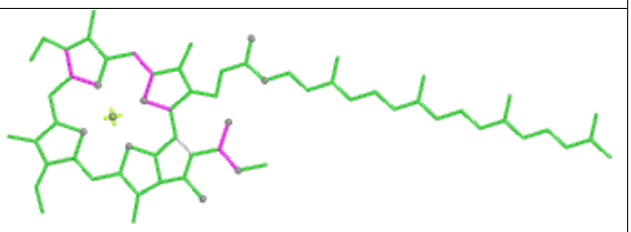
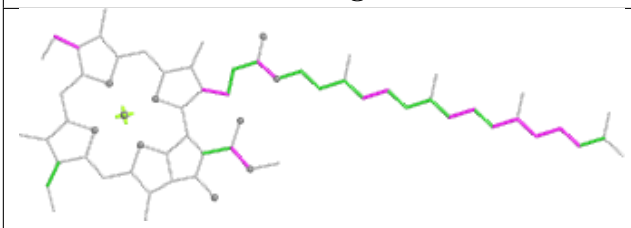
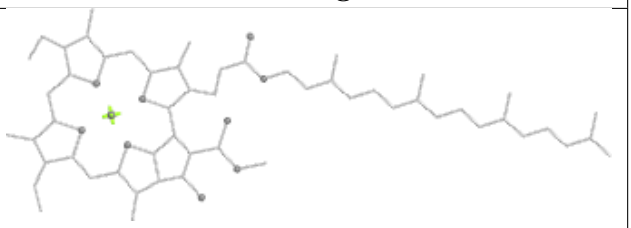
 Bond lengths	 Bond angles
 Torsions	 Rings

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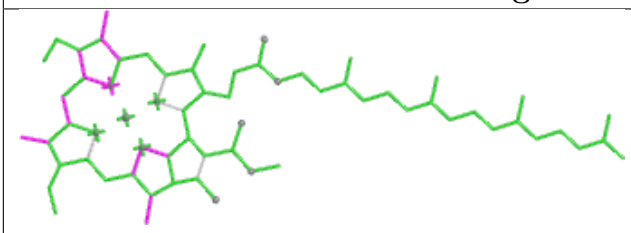
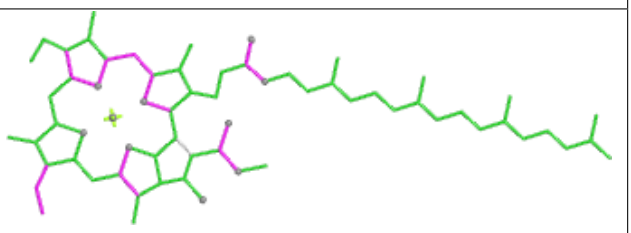
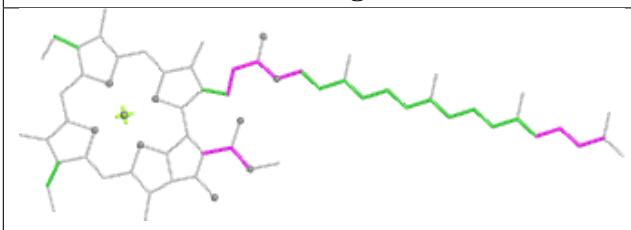
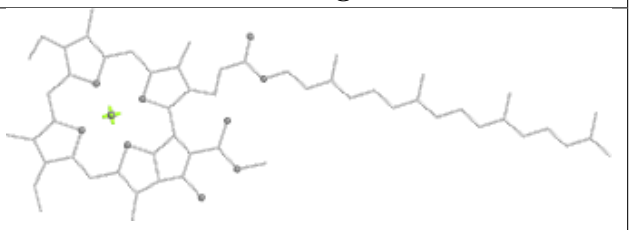
 Bond lengths	 Bond angles
 Torsions	 Rings

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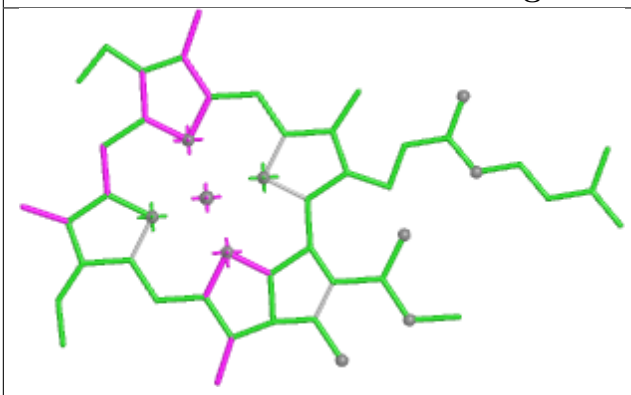
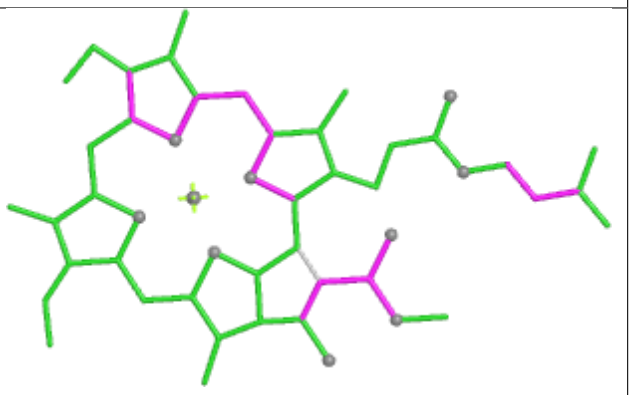
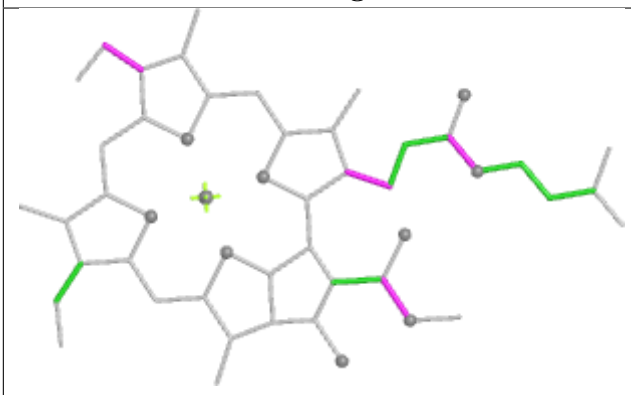
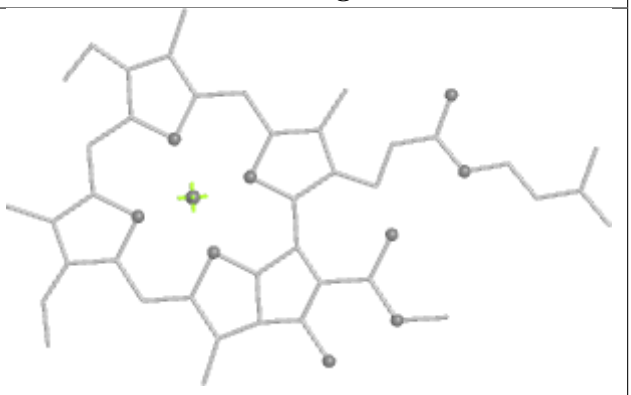
 Bond lengths	 Bond angles
 Torsions	 Rings

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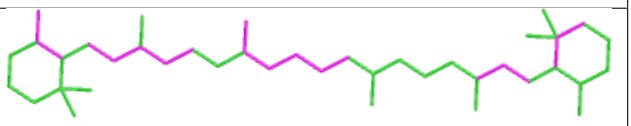
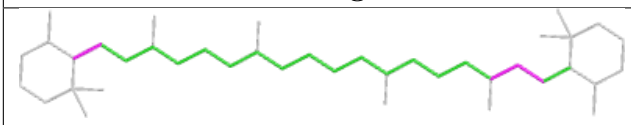
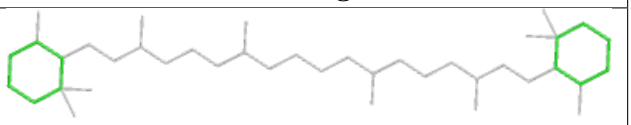
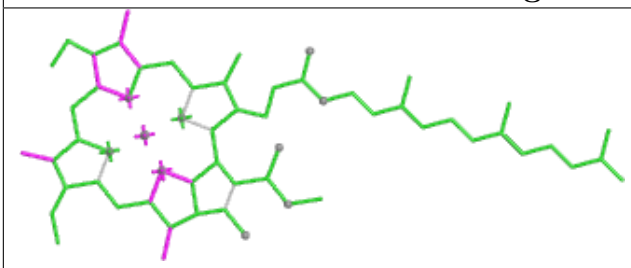
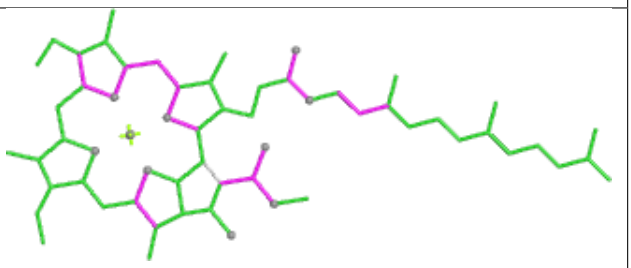
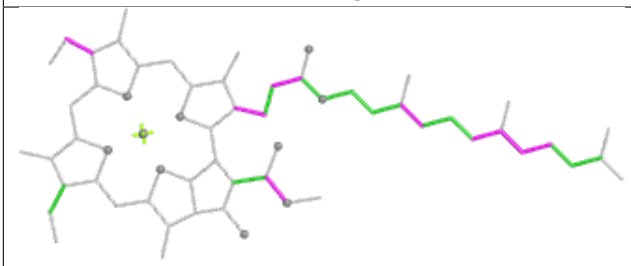
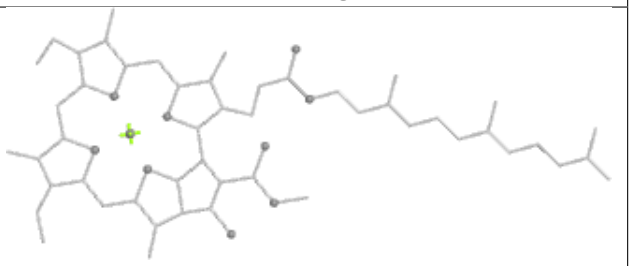
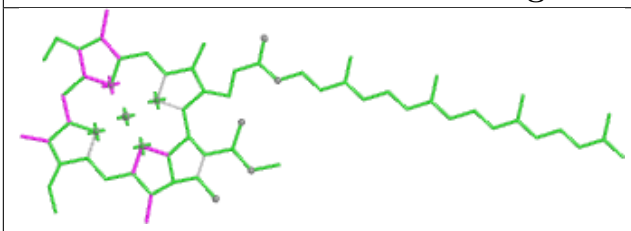
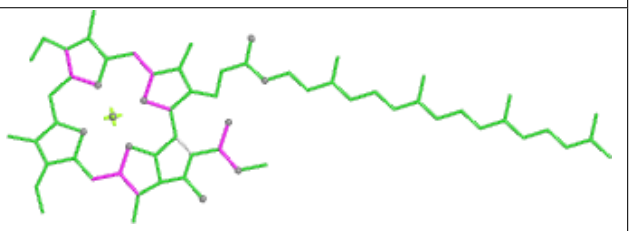
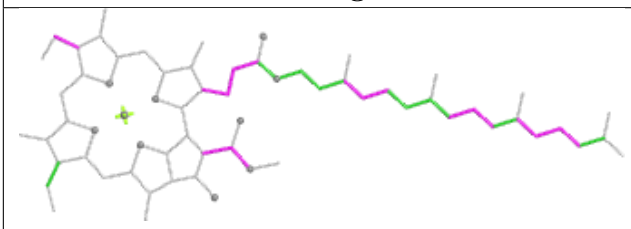
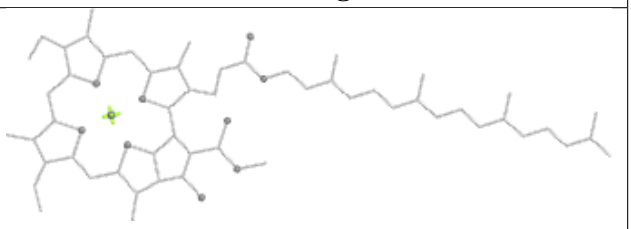
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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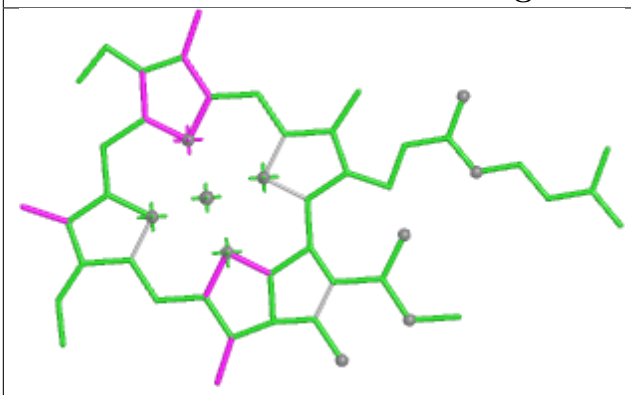
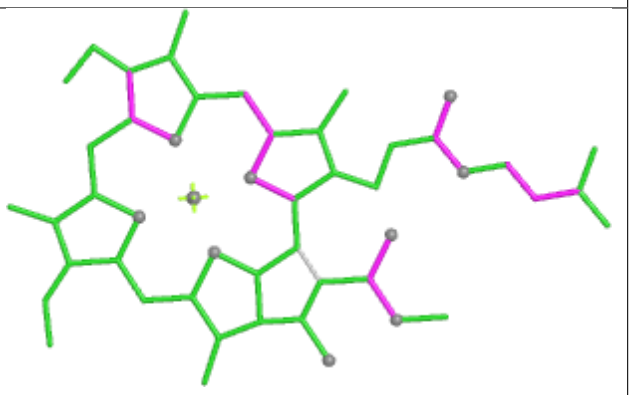
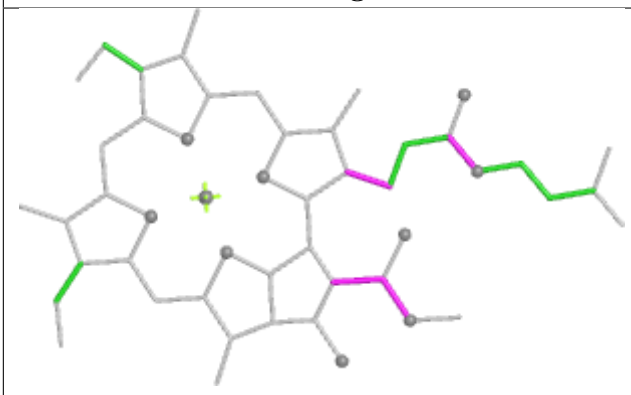
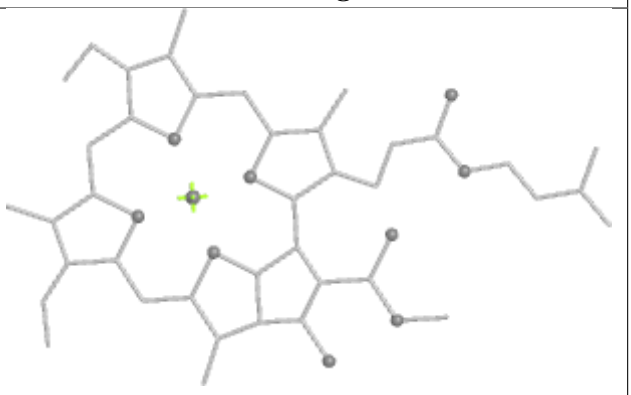
 Bond lengths	 Bond angles
 Torsions	 Rings

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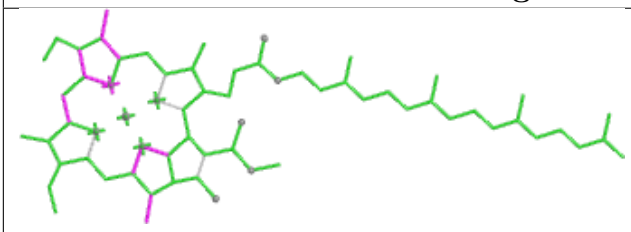
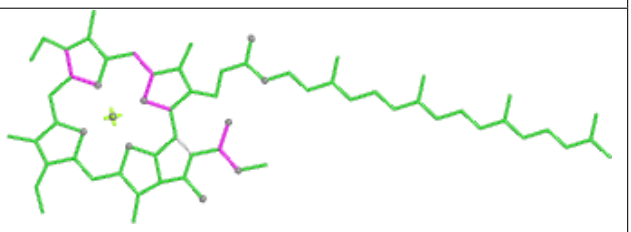
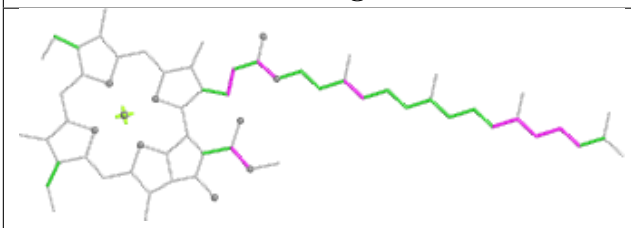
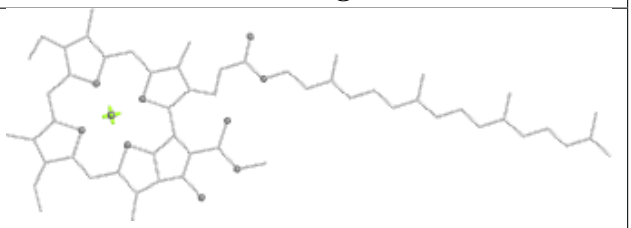
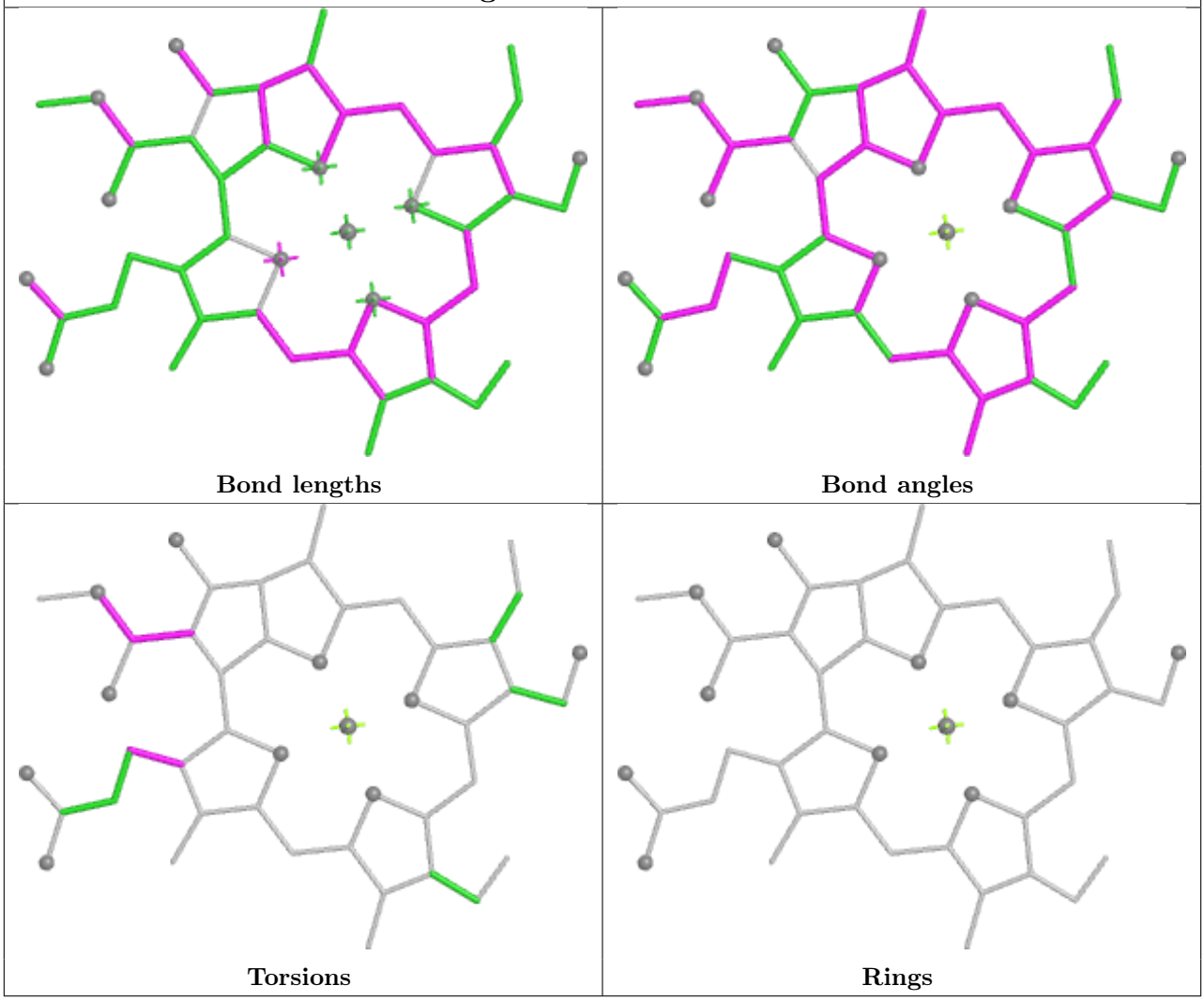
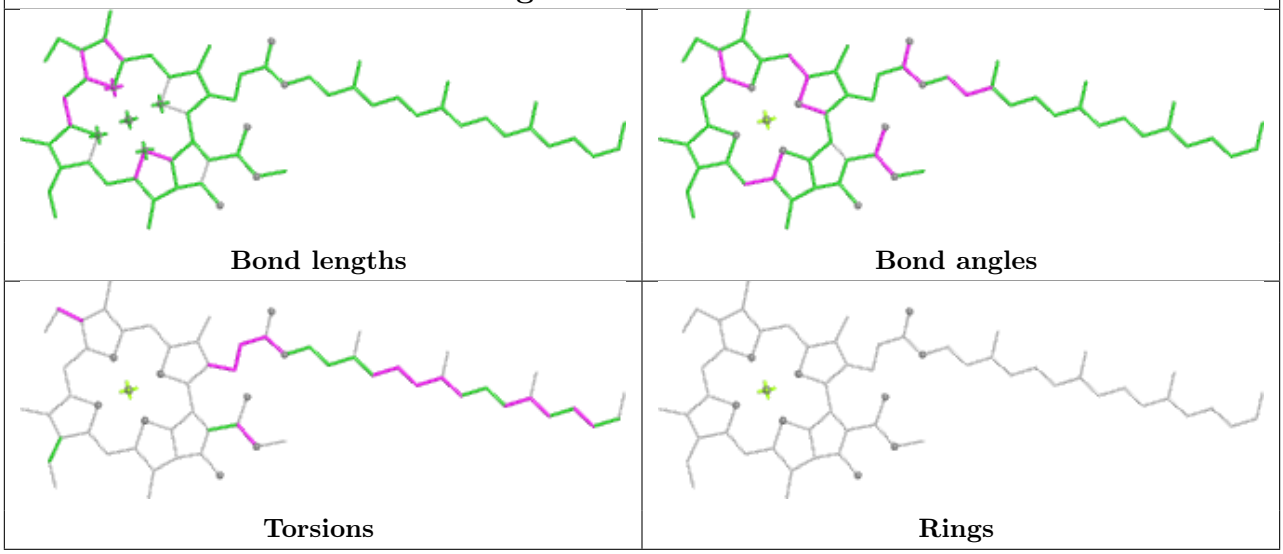
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AB 306



Ligand CLA BJ 610



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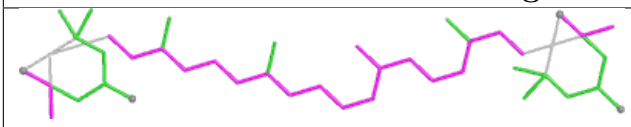
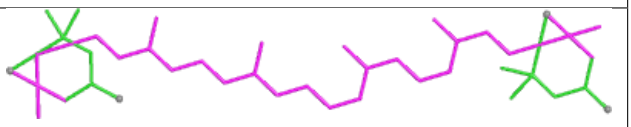
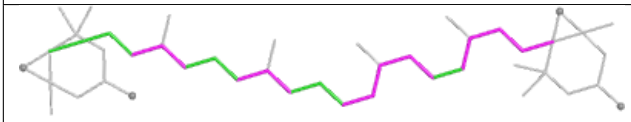
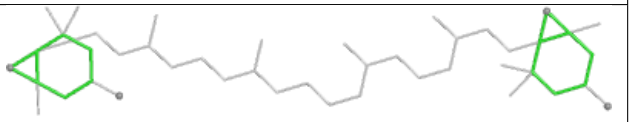
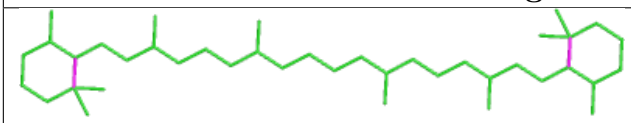
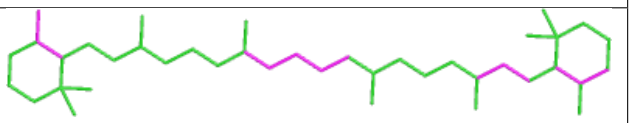
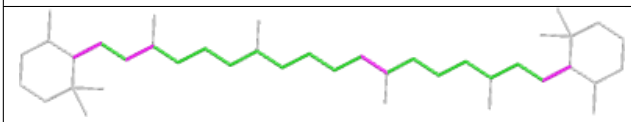
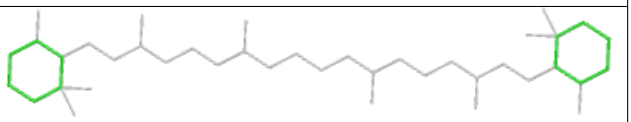
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

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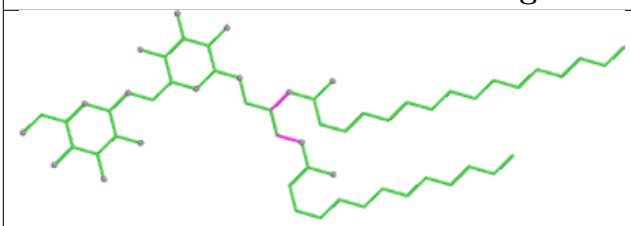
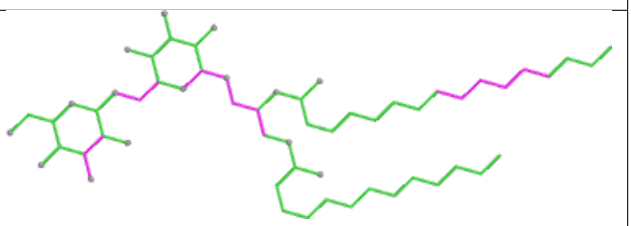
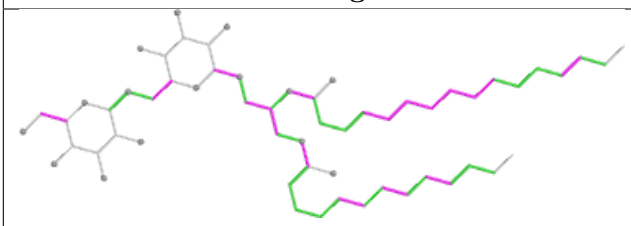
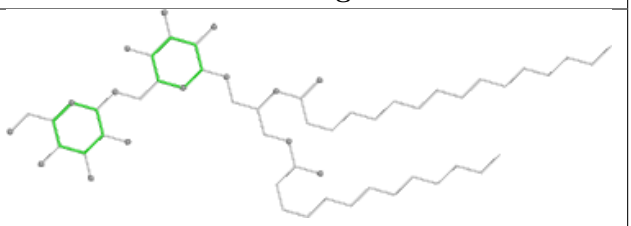
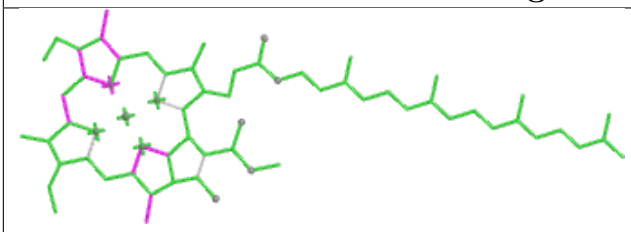
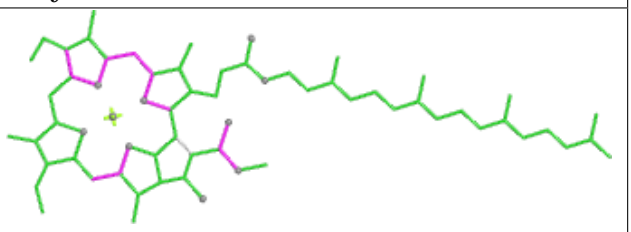
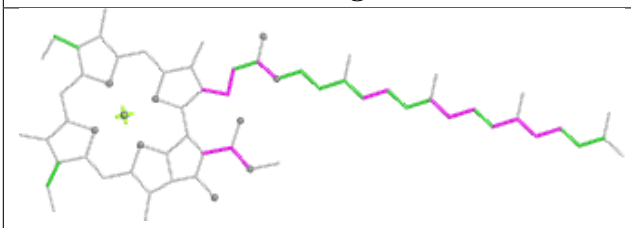
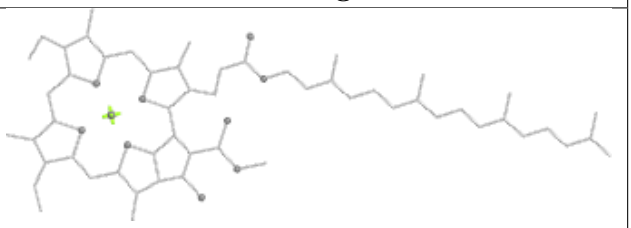
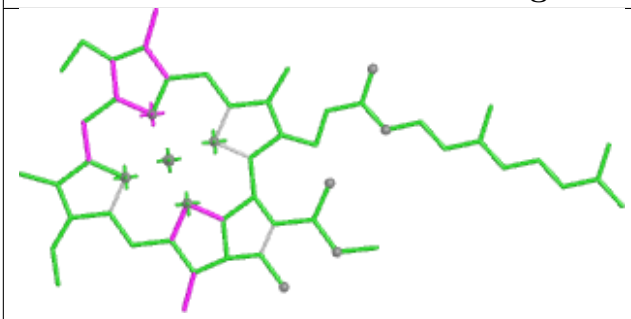
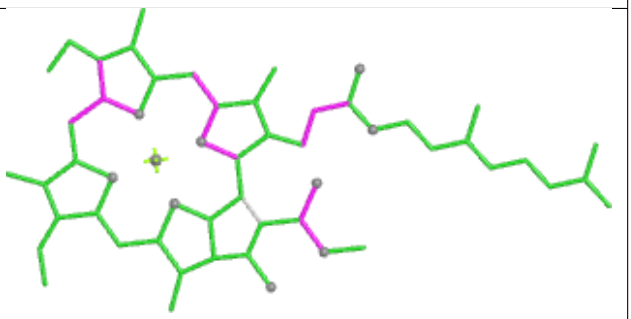
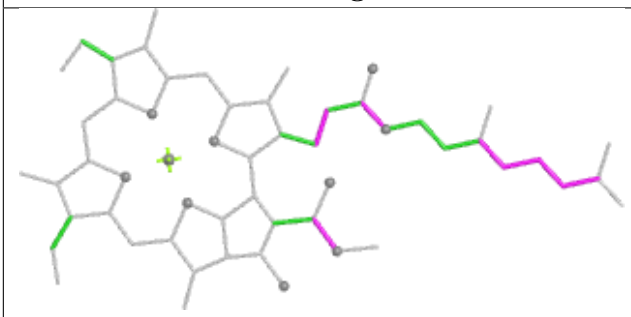
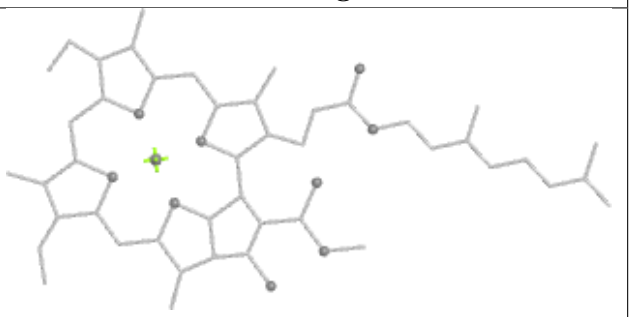
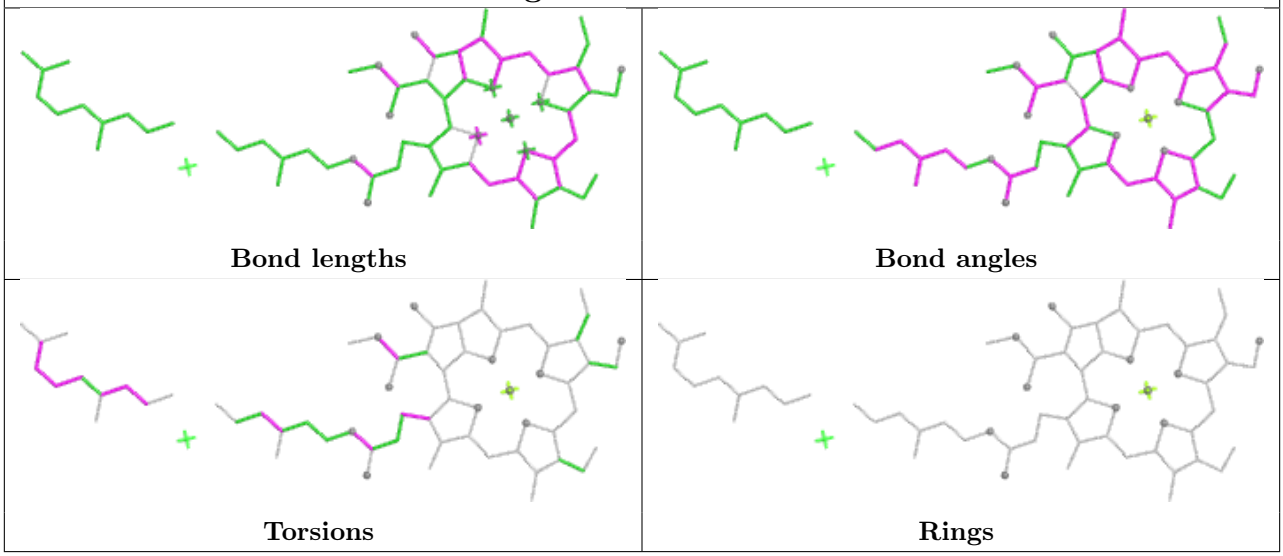
 Bond lengths	 Bond angles
 Torsions	 Rings

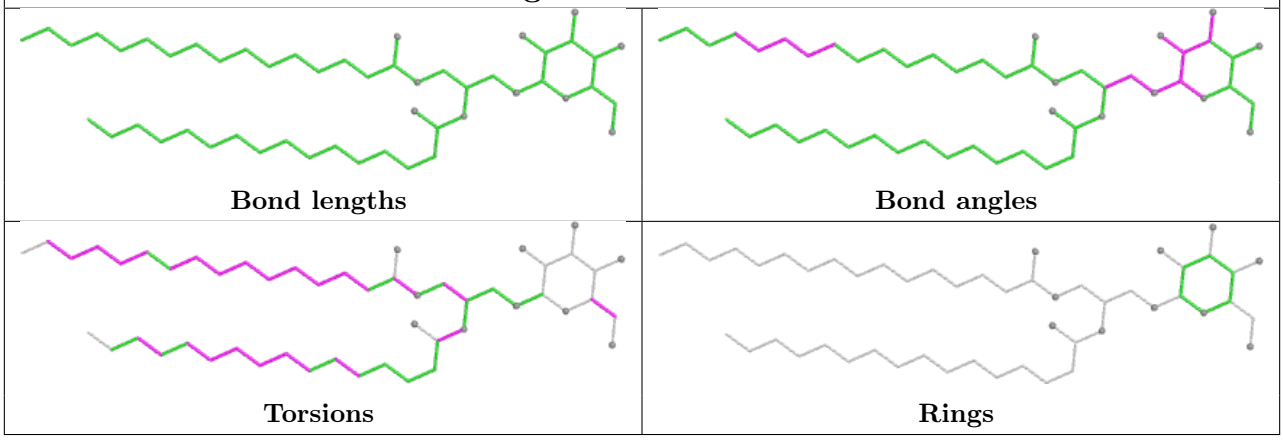
Ligand CLA y 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

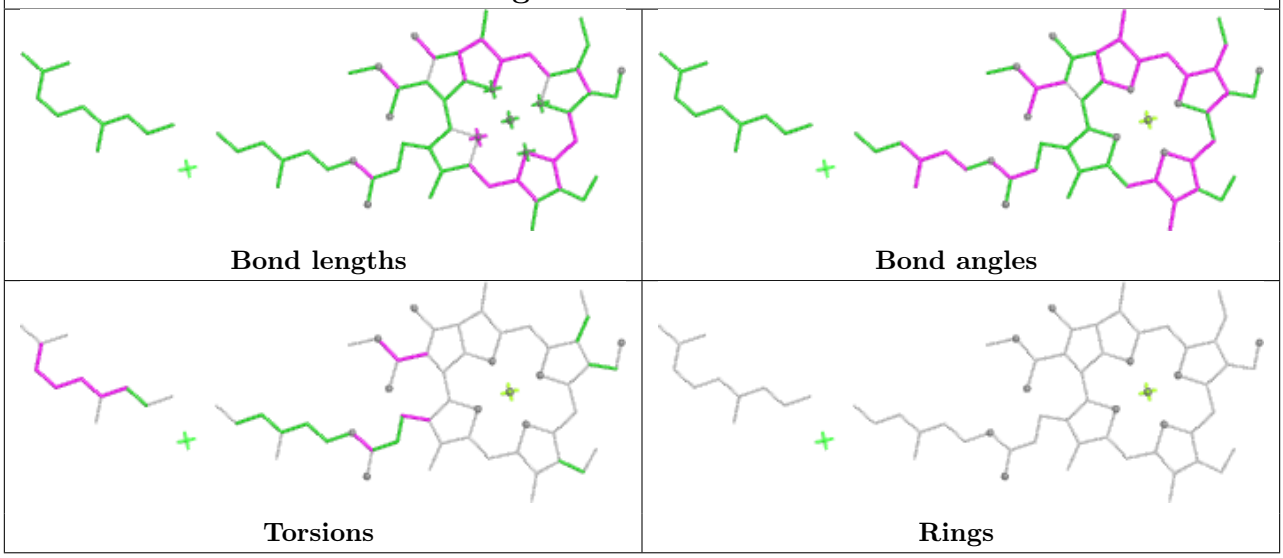
Ligand CHL Y 302



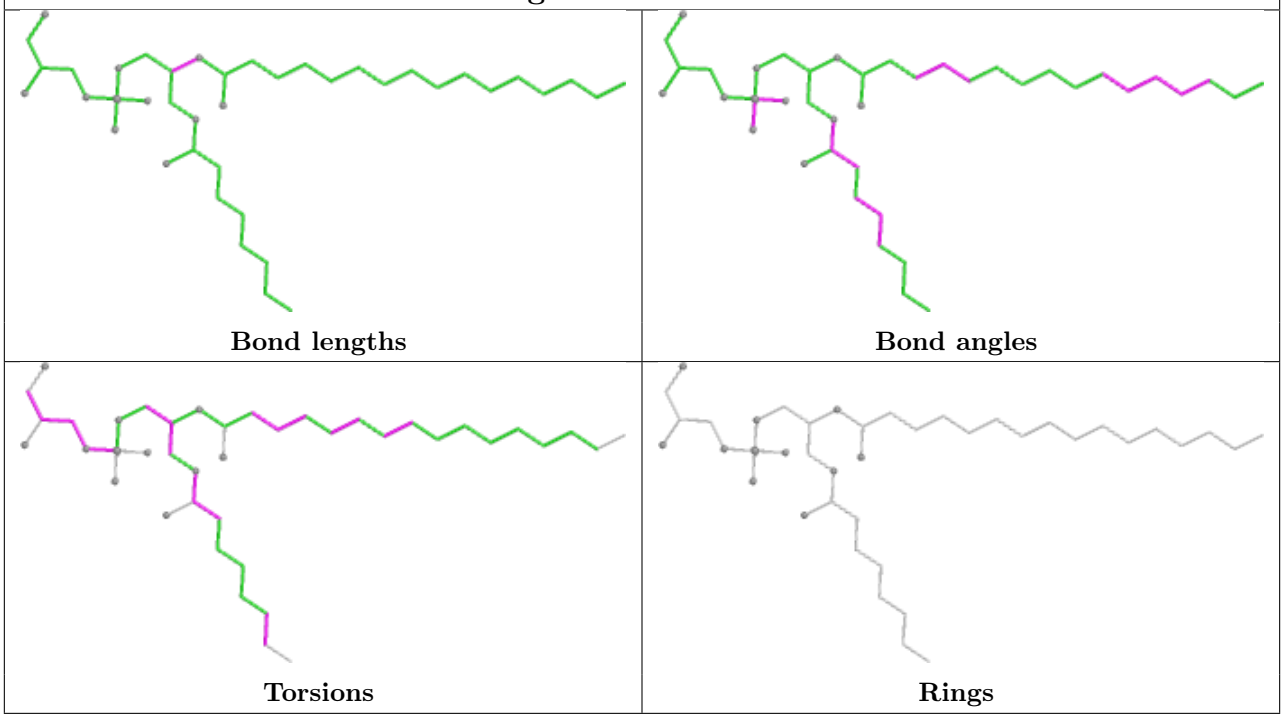
Ligand LMG b 621



Ligand CHL BB 310



Ligand LHG 5 618



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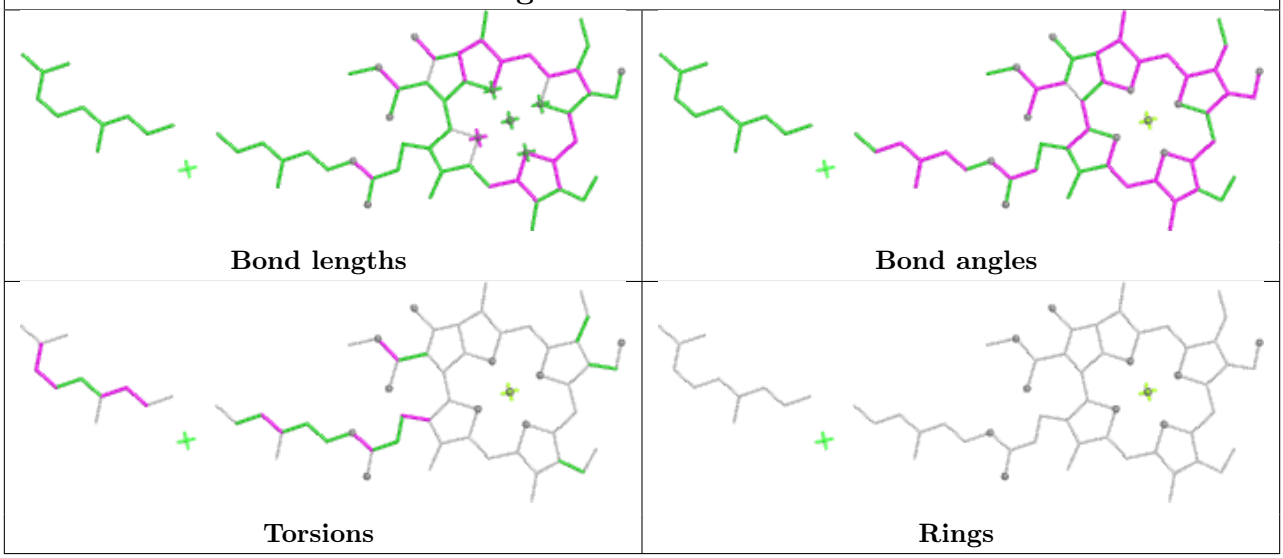

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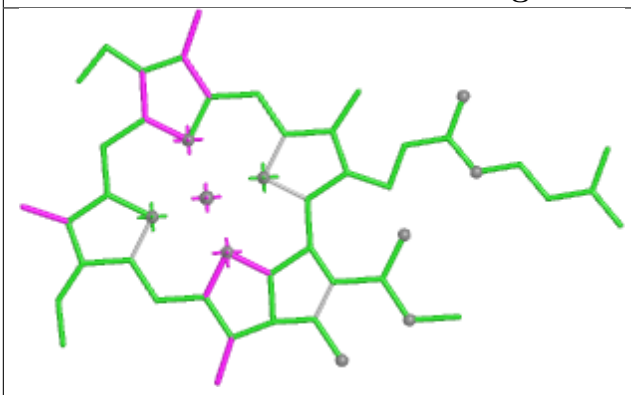
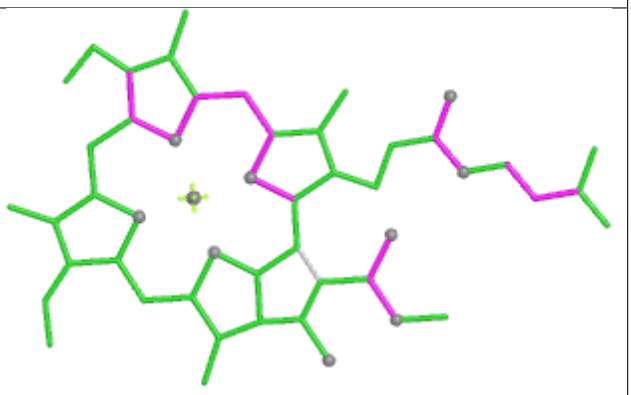
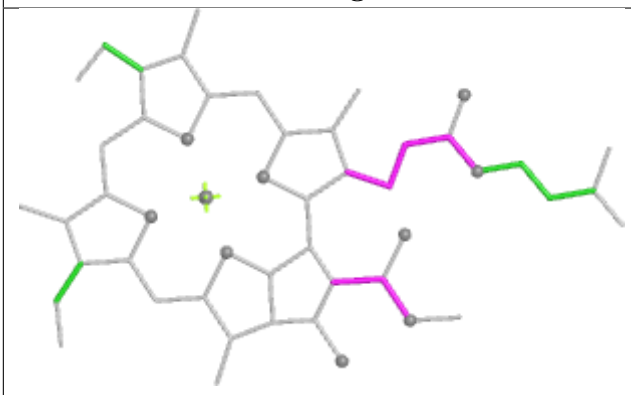
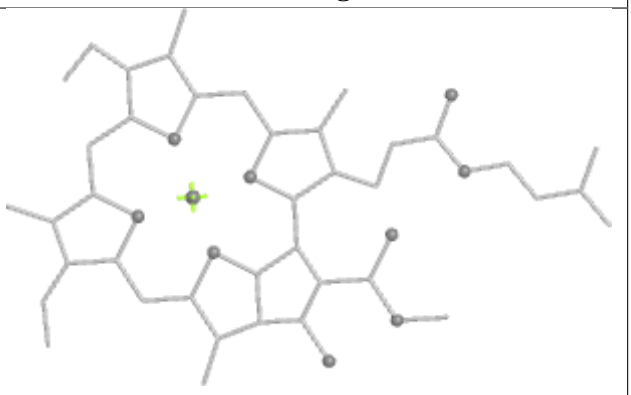
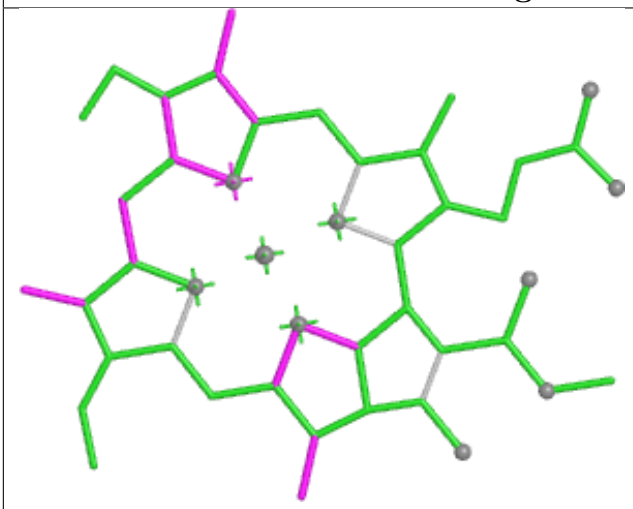
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A6 603



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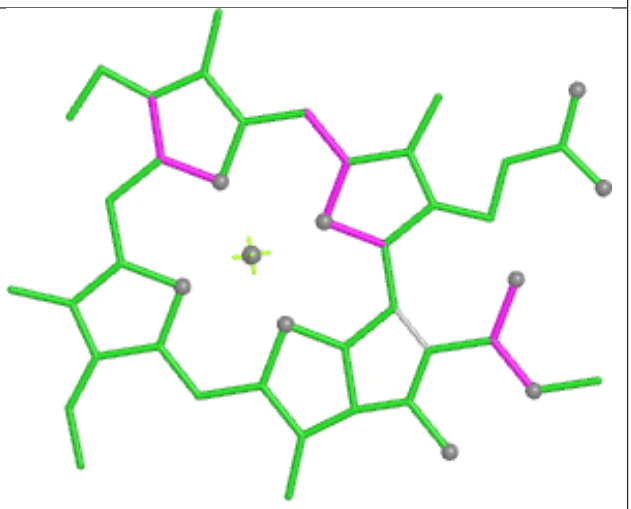

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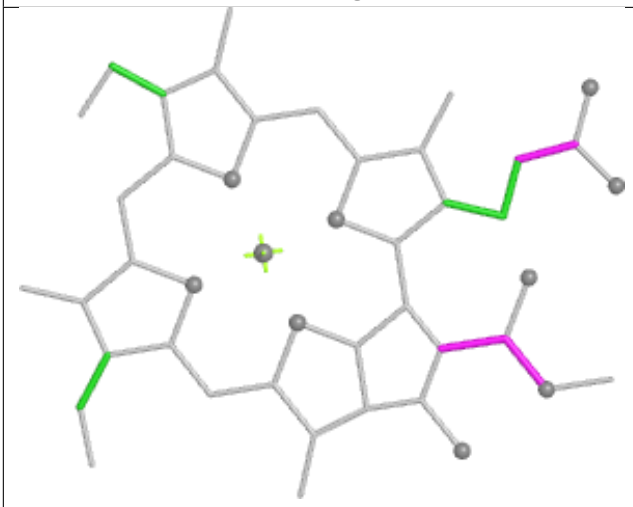
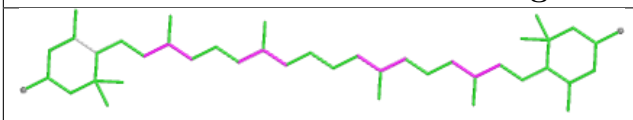


Torsions

Rings

Ligand LUT s 614



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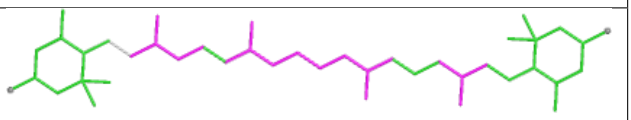

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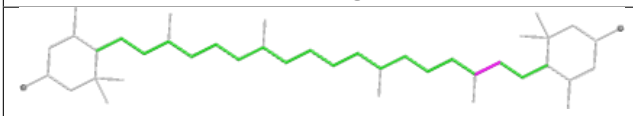

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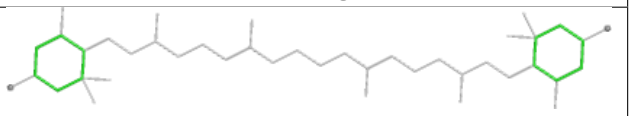

Rings

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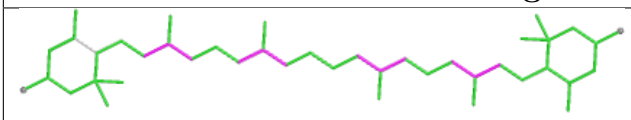

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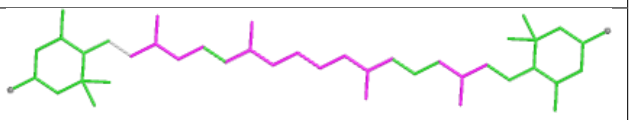

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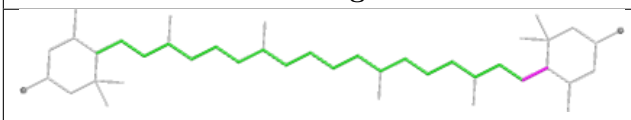

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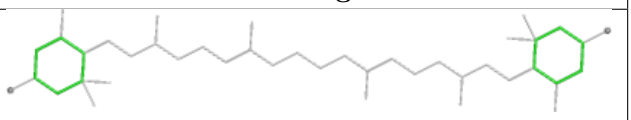
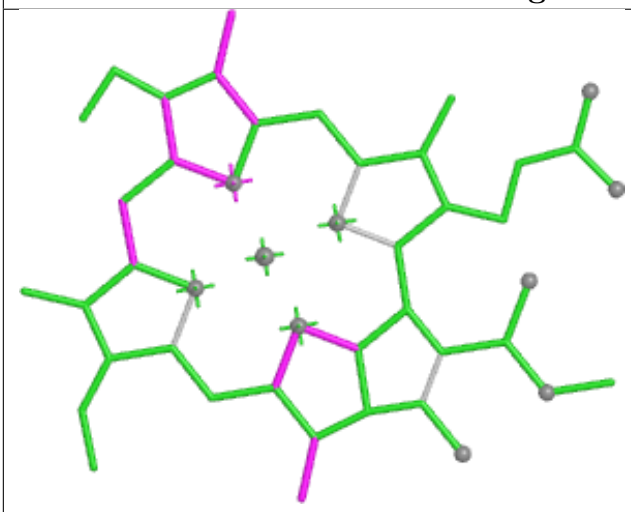


Rings

Ligand CLA 8 310



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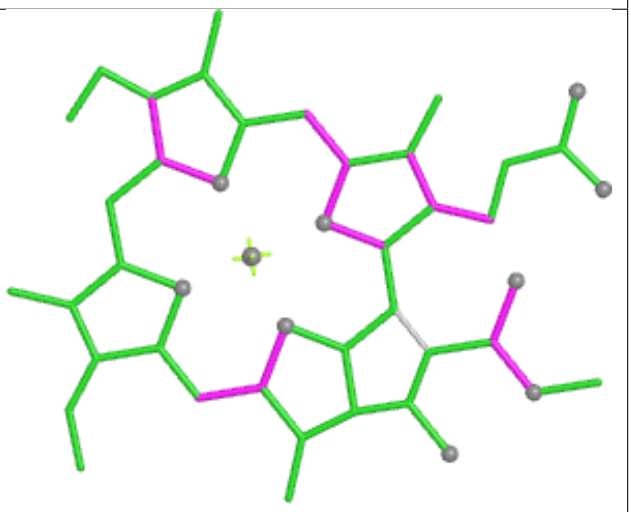

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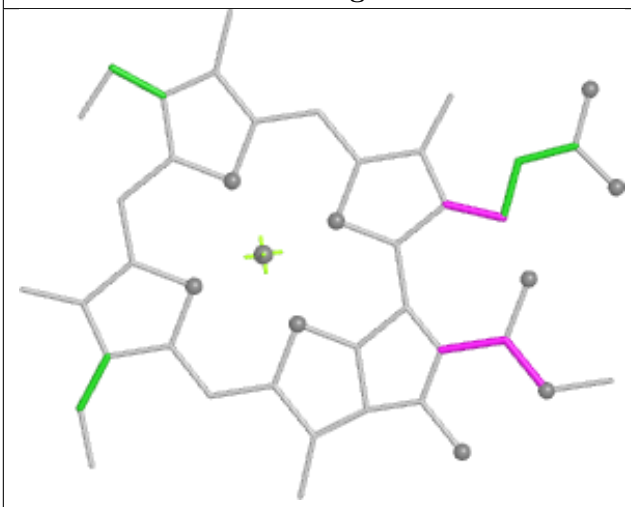

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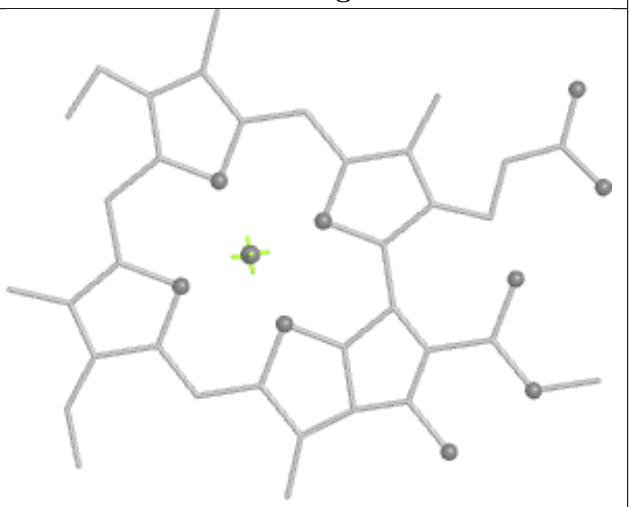
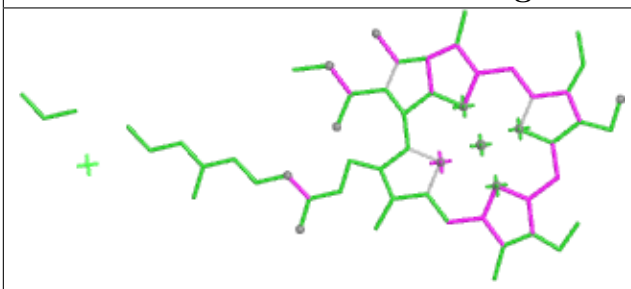
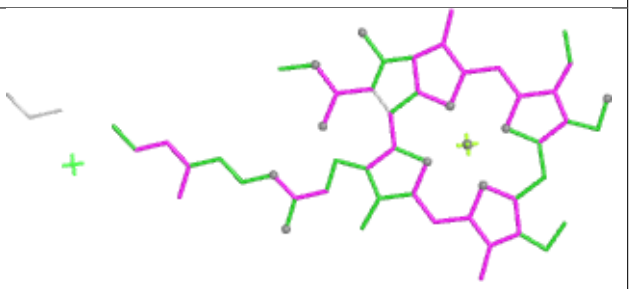
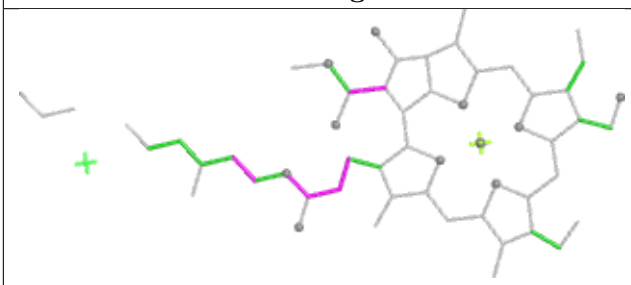
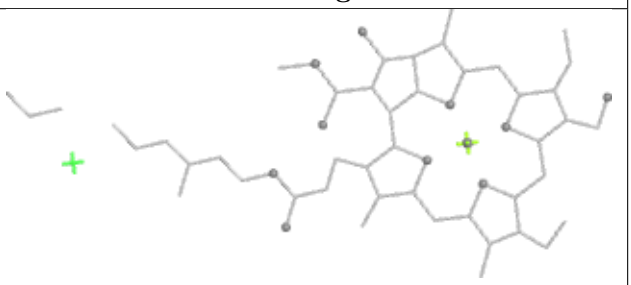
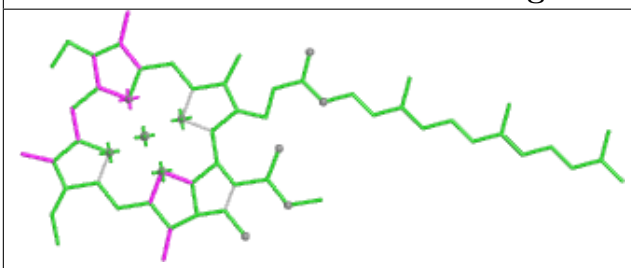
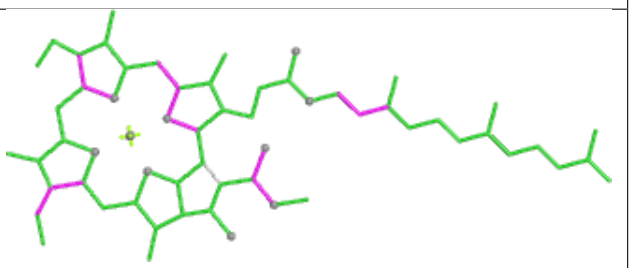
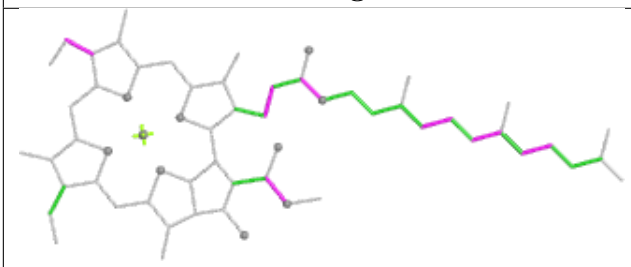
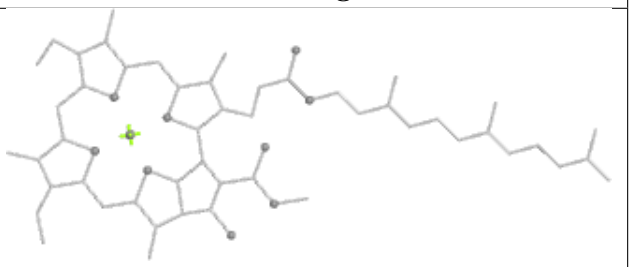


Rings

Ligand CHL A6 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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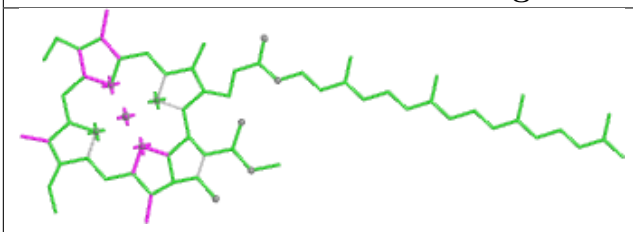

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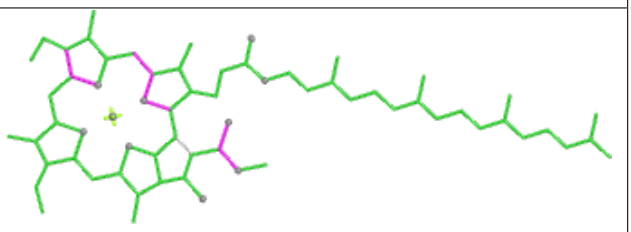

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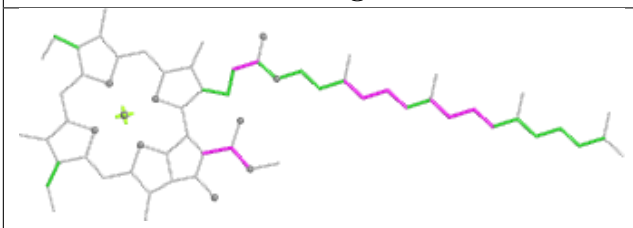

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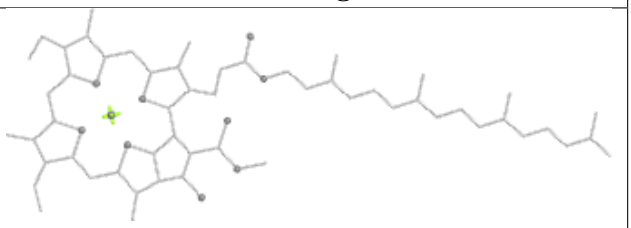
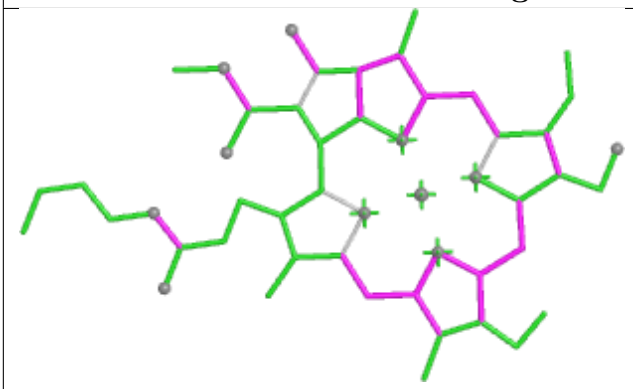


Rings

Ligand CHL BB 307



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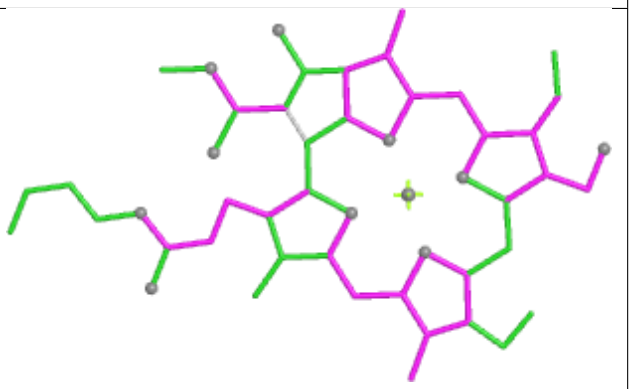

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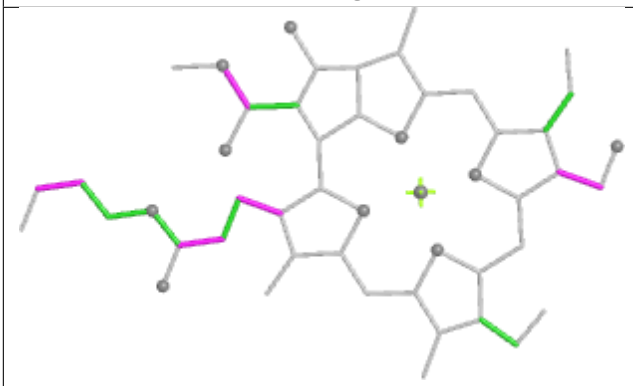
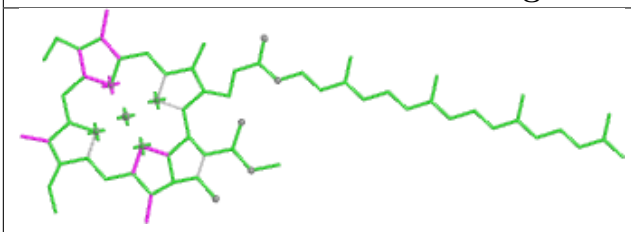
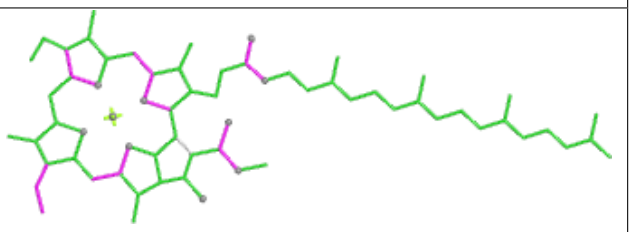
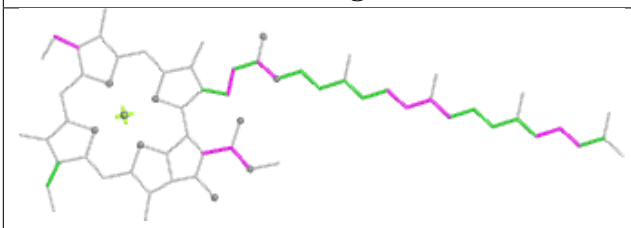
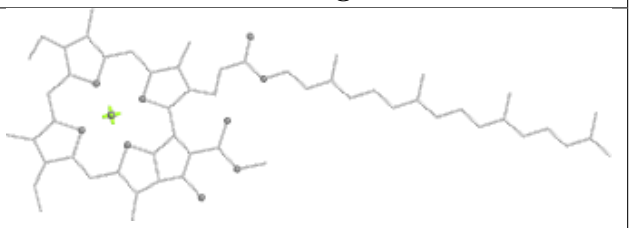


Torsions

Rings

Ligand CLA G 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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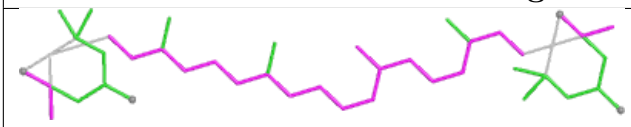
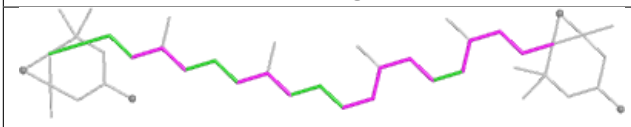
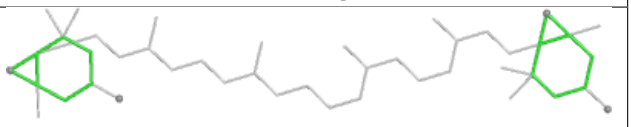
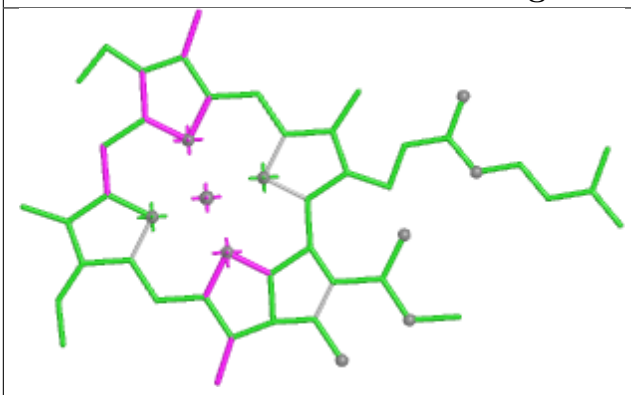
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA 5 604



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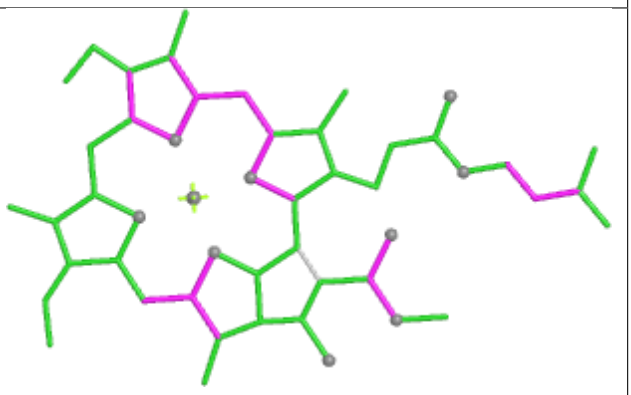

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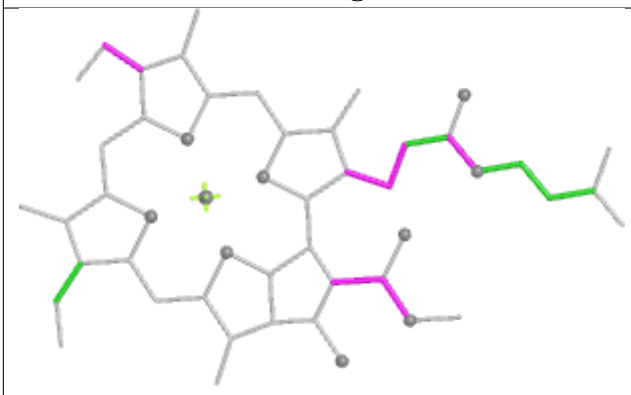

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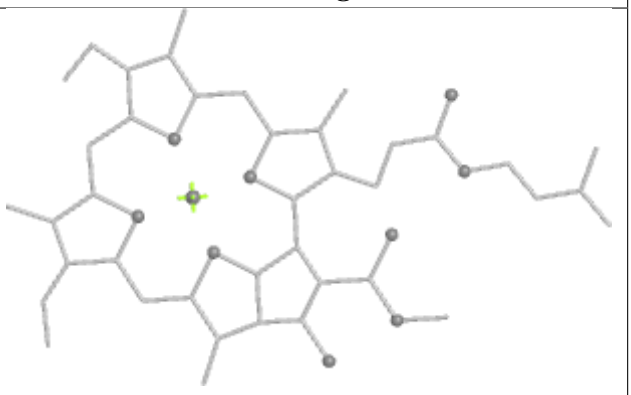


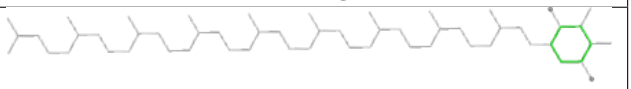
Rings

Ligand PL9 D 403

Bond lengths

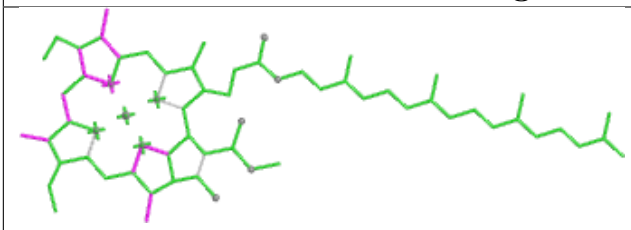
Bond angles

Torsions

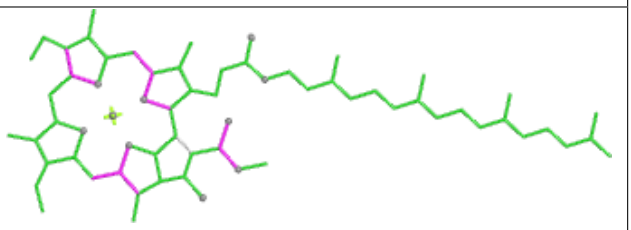


Rings

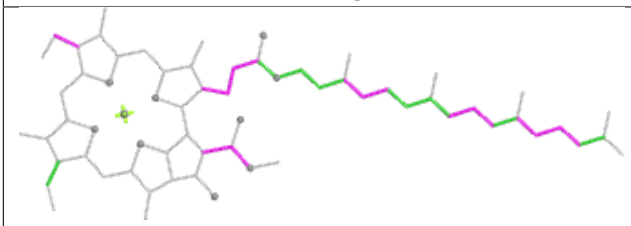
Ligand CLA BE 606



Bond lengths



Bond angles



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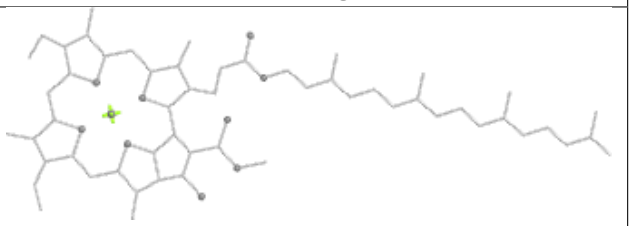
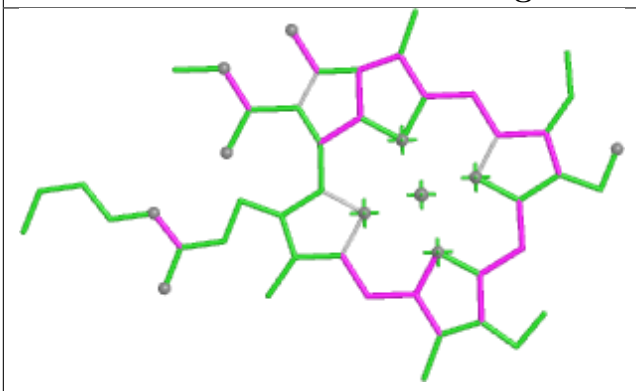
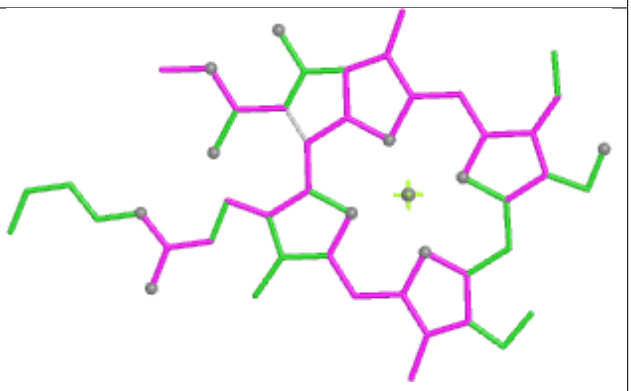
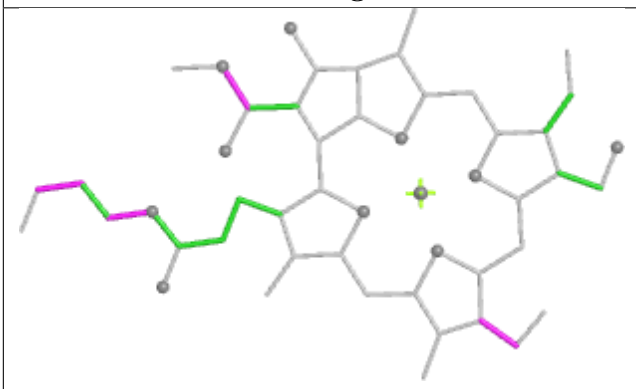
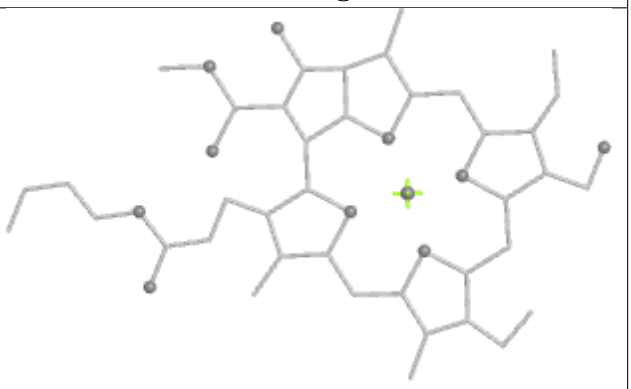
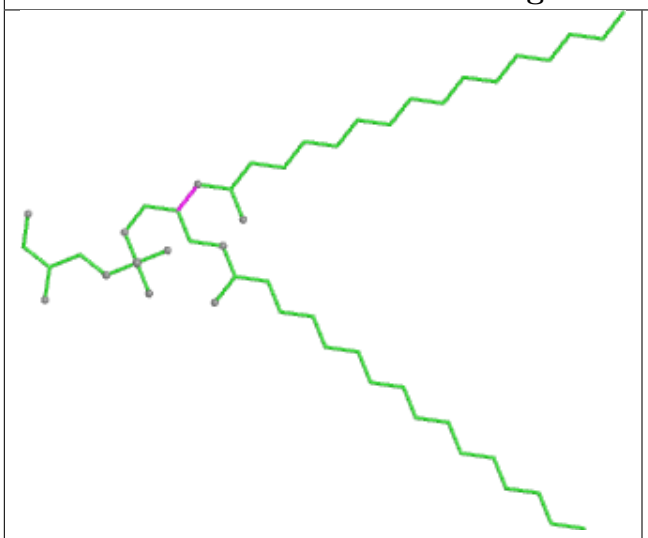


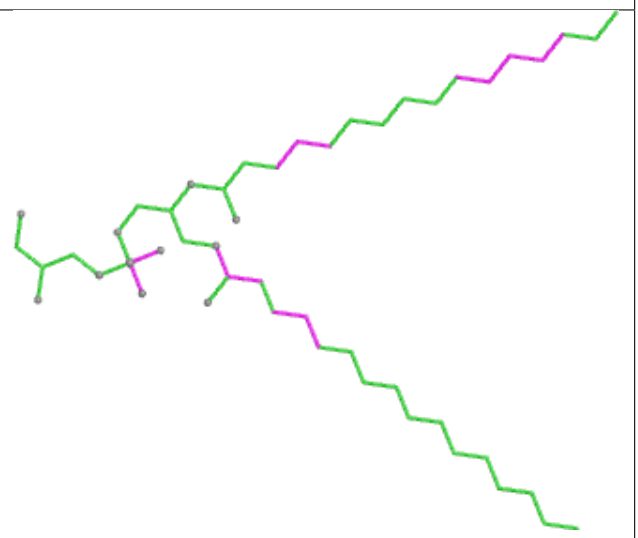
Rings

Ligand CHL BJ 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

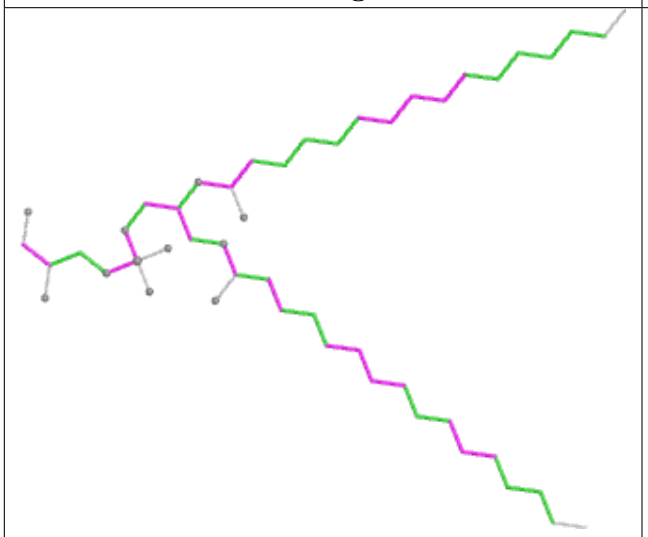
Ligand LHG b 622



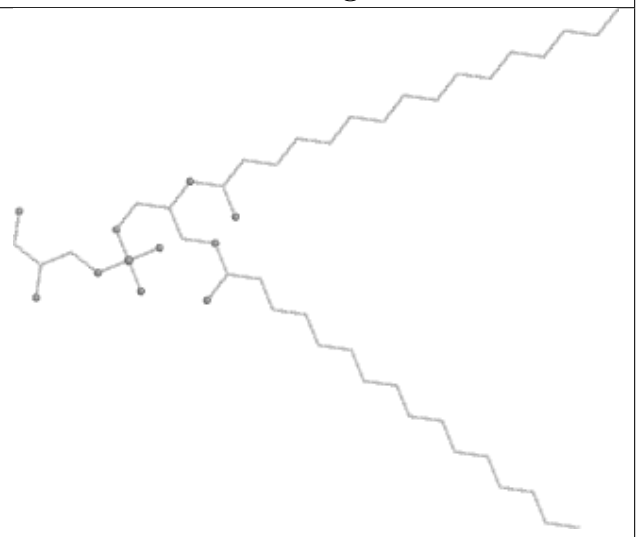
Bond lengths



Bond angles

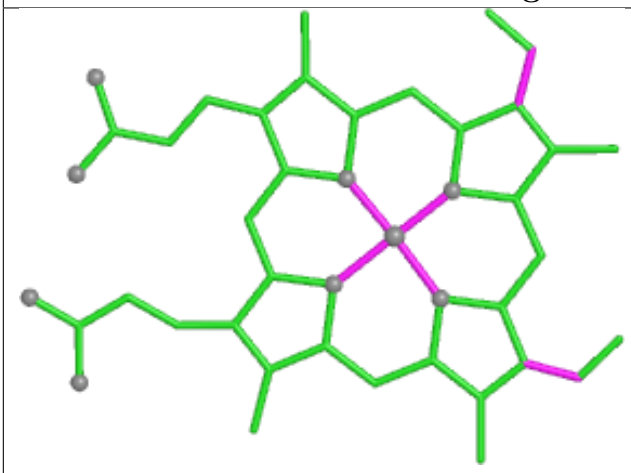


Torsions



Rings

Ligand HEM 4 102



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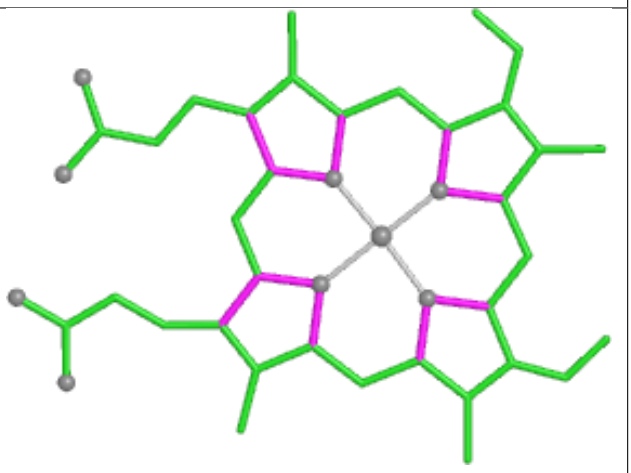
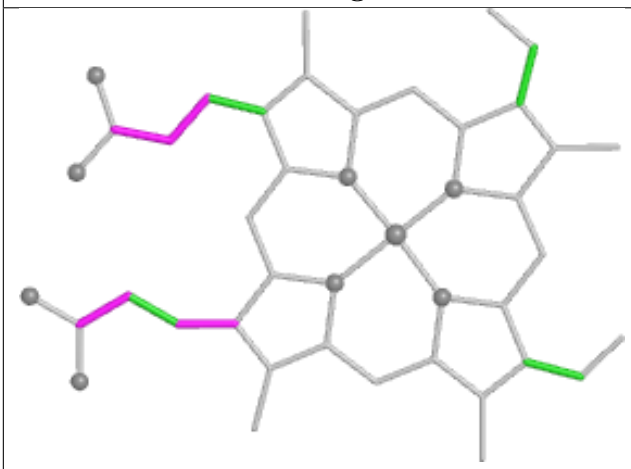
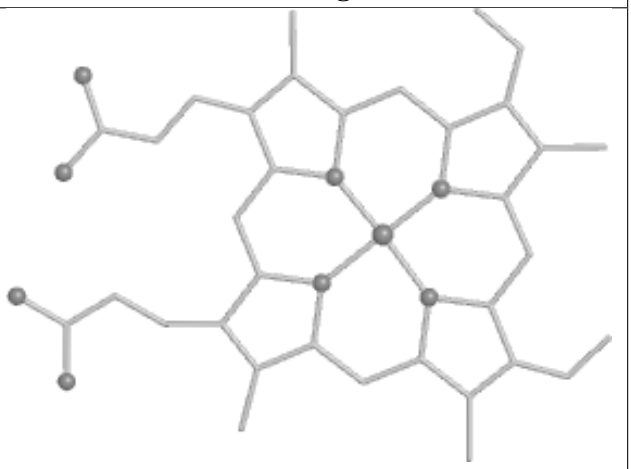


Bond angles

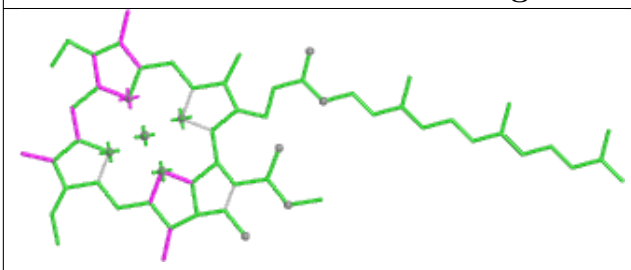


Torsions

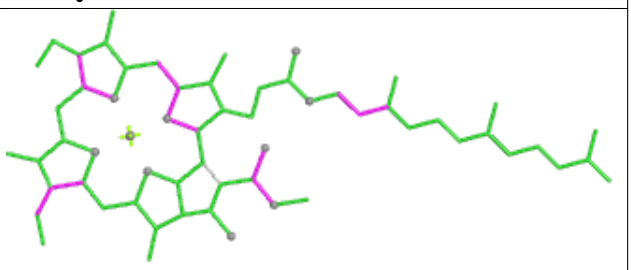


Rings

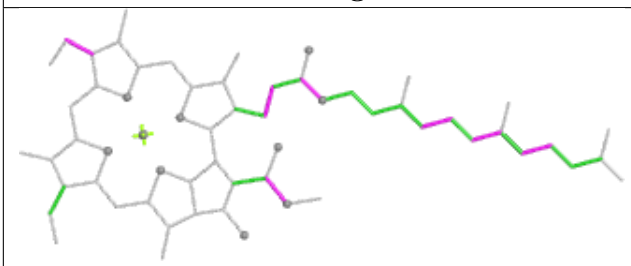
Ligand CLA BQ 613



Bond lengths



Bond angles



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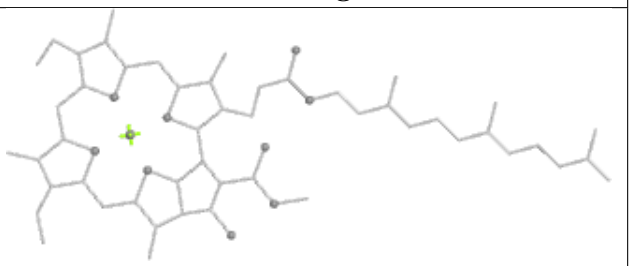
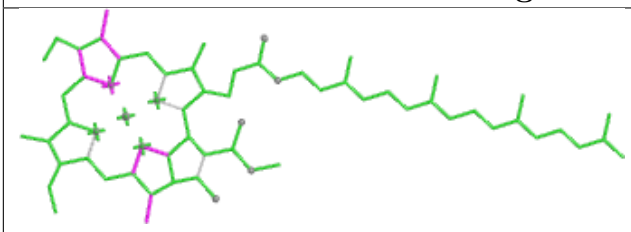
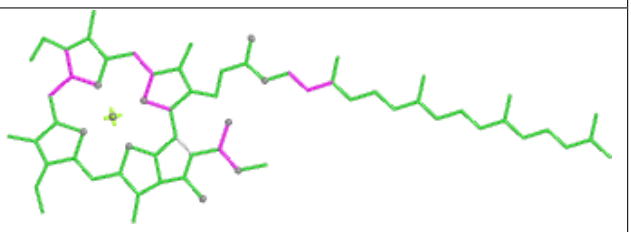
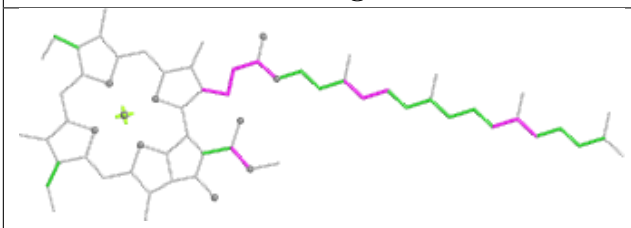
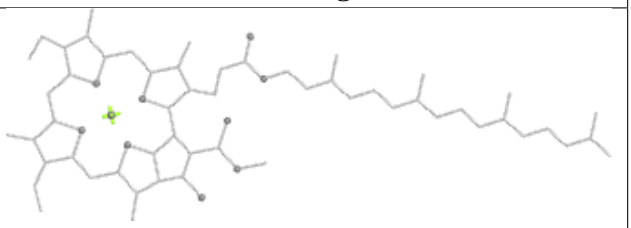
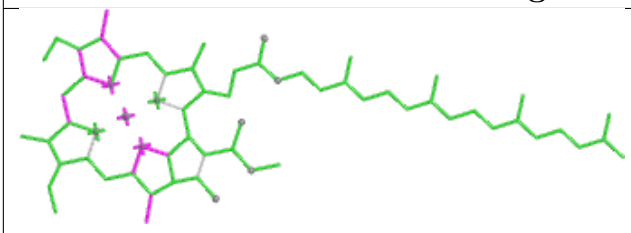
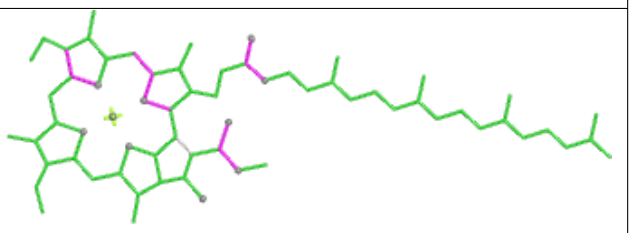
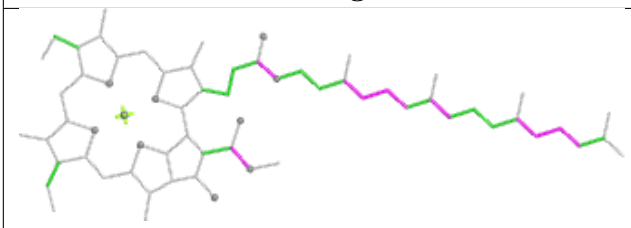
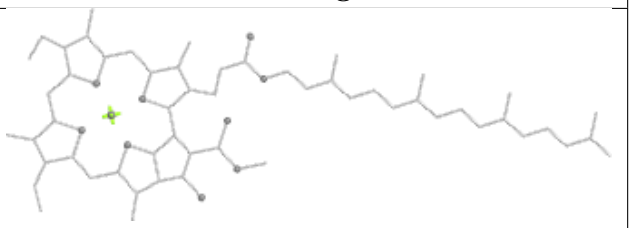
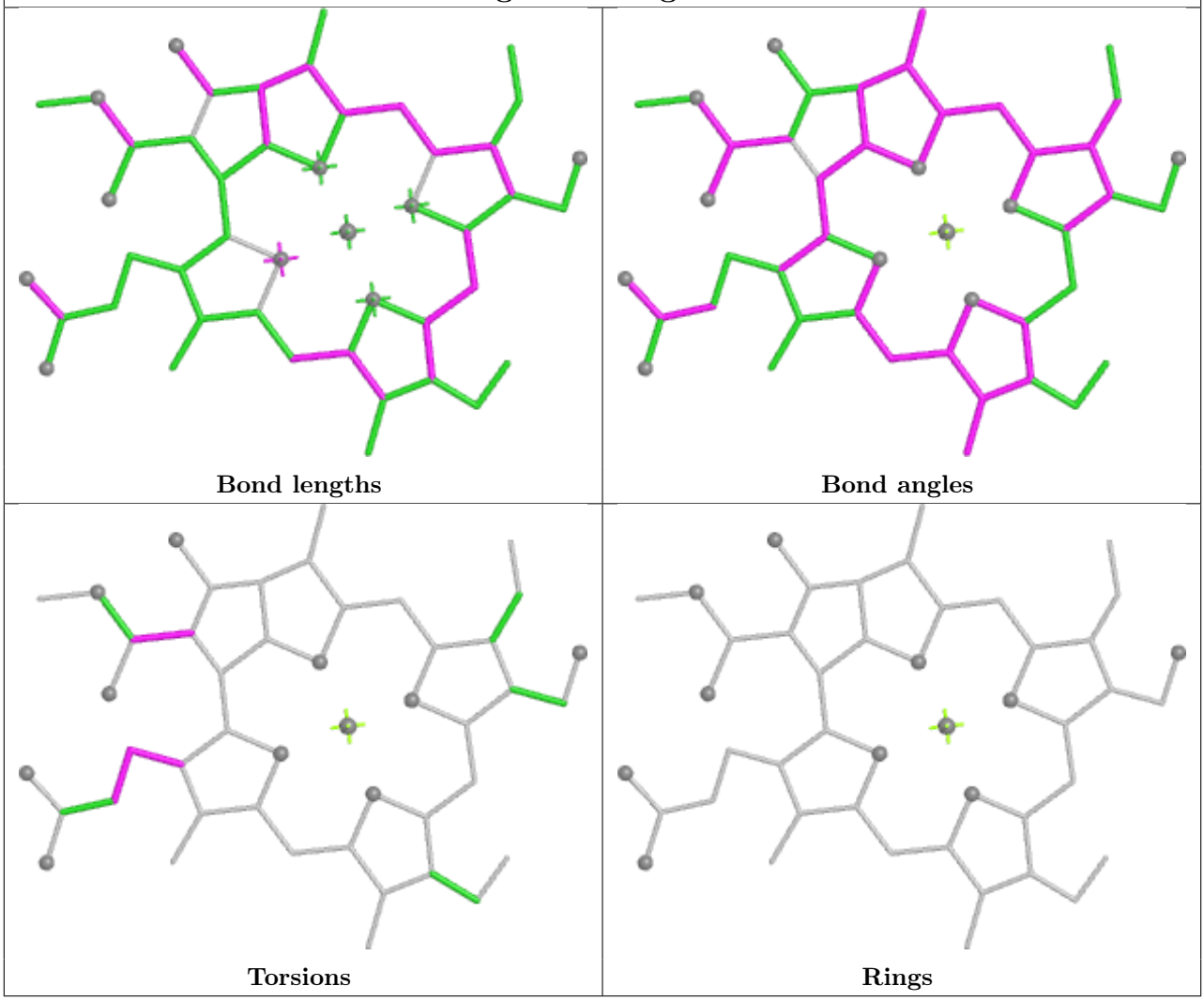


Rings

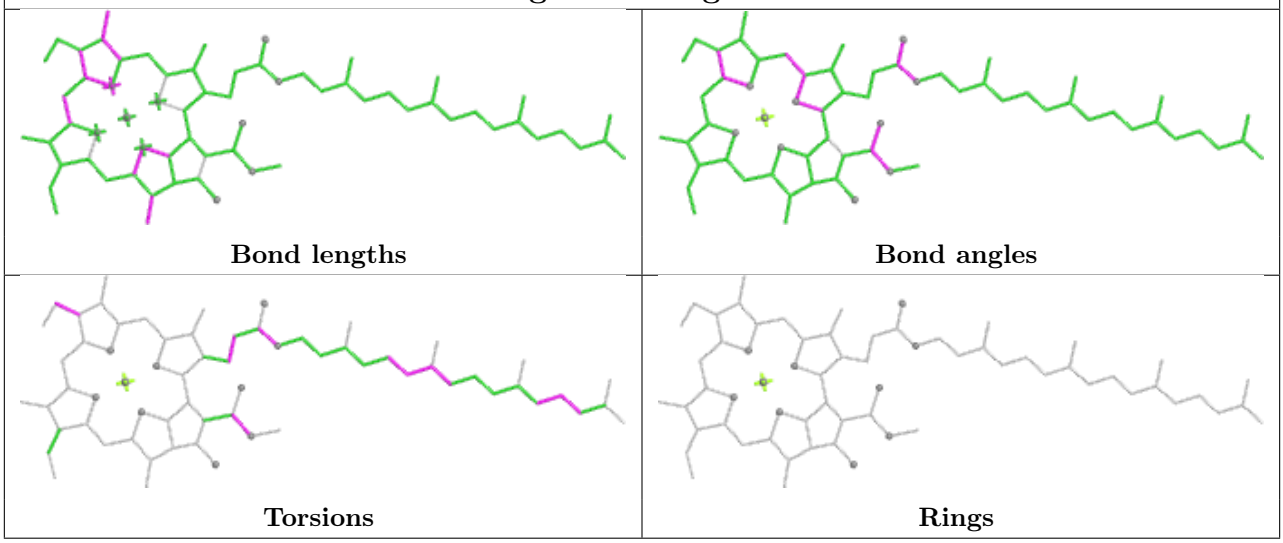
Ligand CLA Ba 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

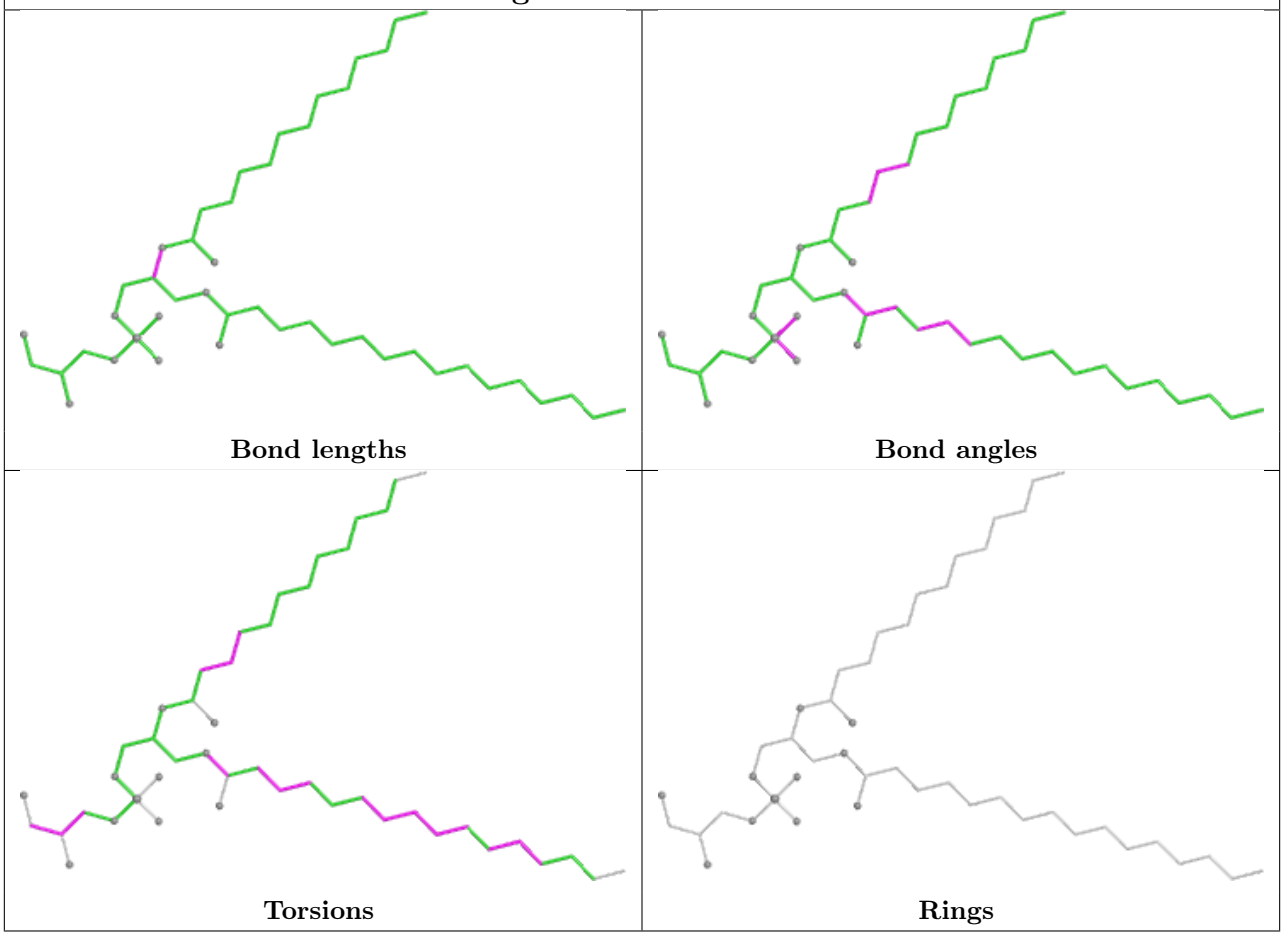
Ligand CHL g 605



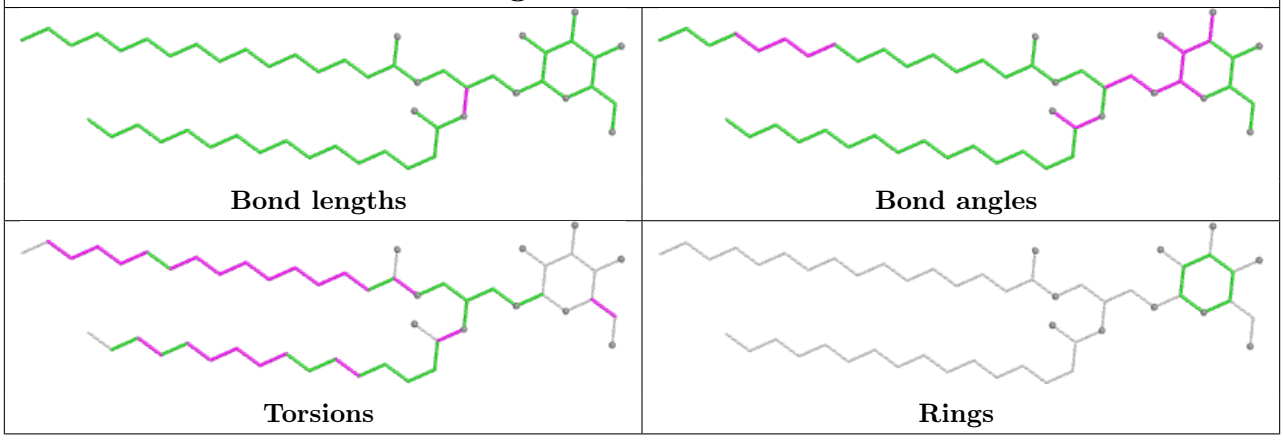
Ligand CLA g 603

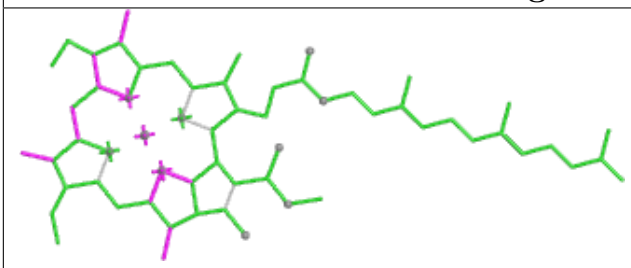
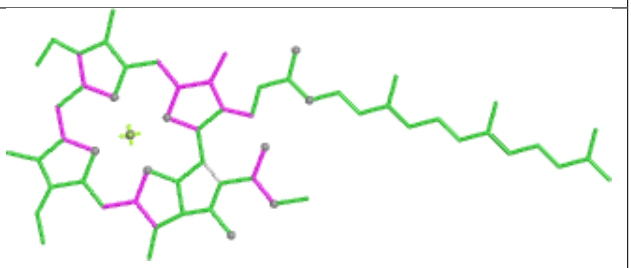
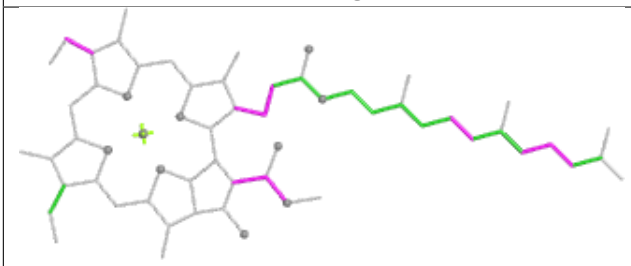
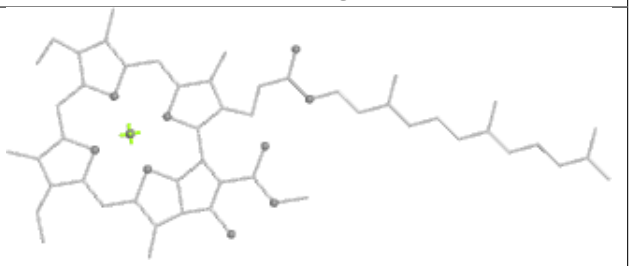


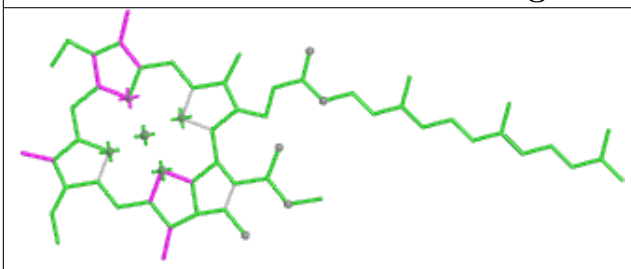
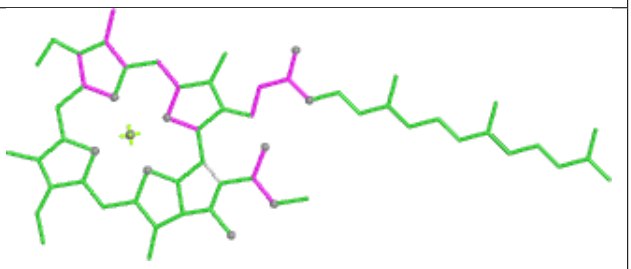
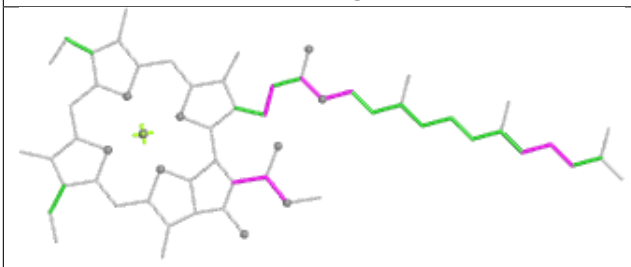
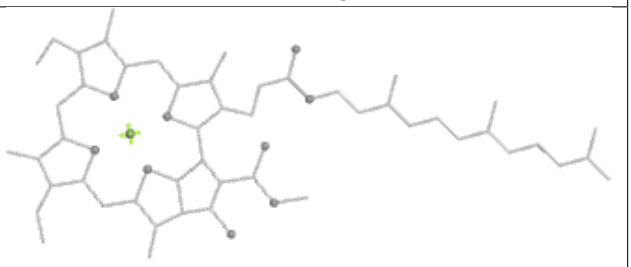
Ligand LHG BE 623



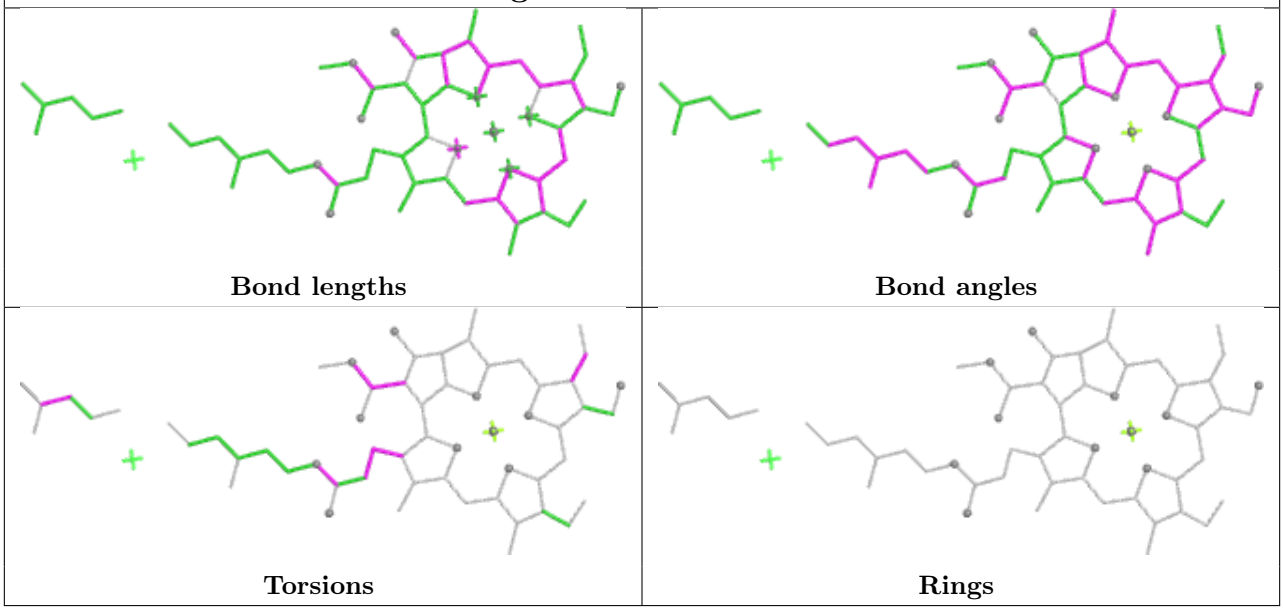
Ligand LMG BE 621



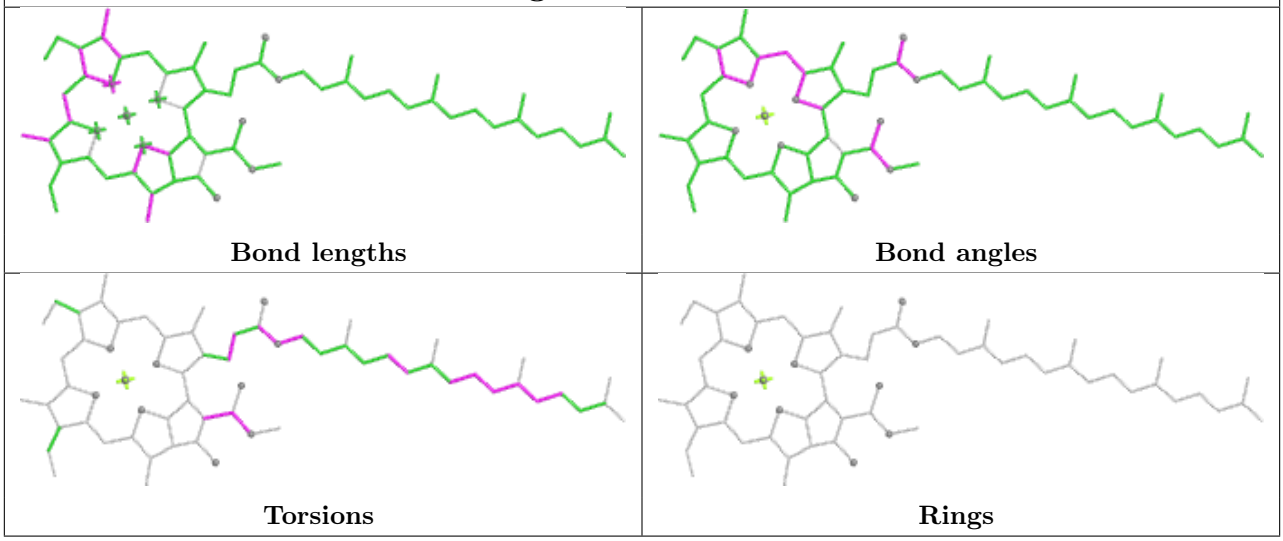
Ligand CLA 6 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

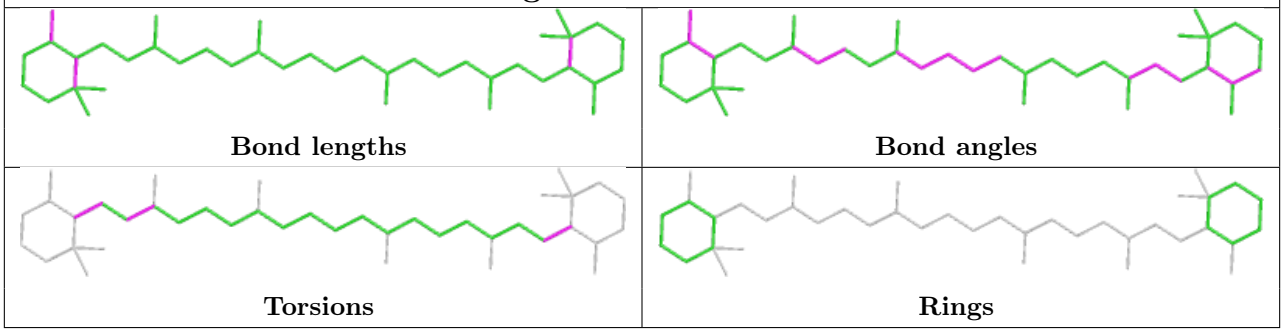
Ligand CHL AA 310



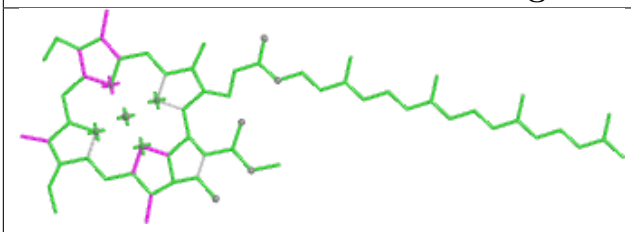
Ligand CLA b 607



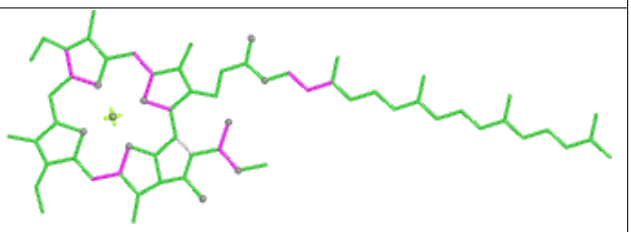
Ligand BCR A 411



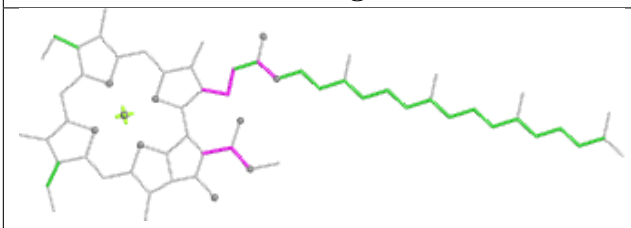
Ligand CLA a 406



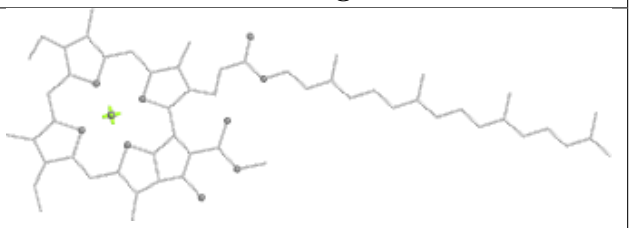
Bond lengths



Bond angles

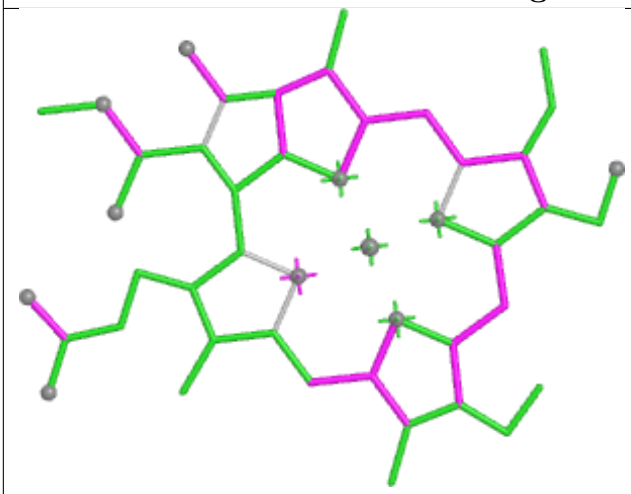


Torsions



Rings

Ligand CHL s 605



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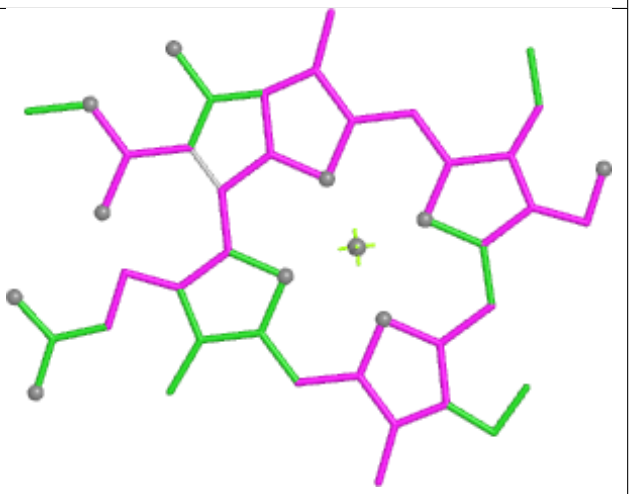
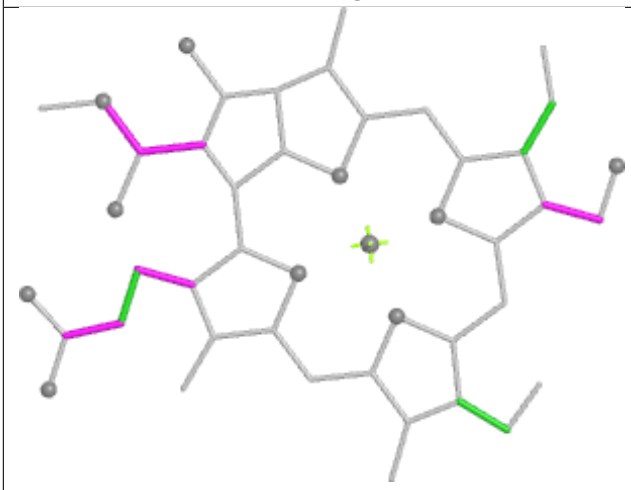
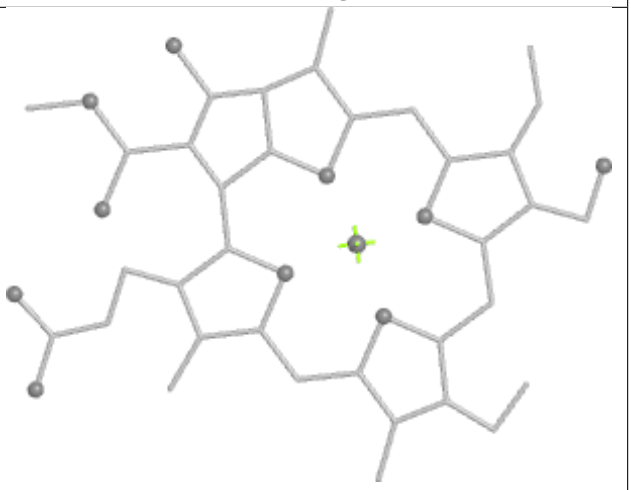


Bond angles

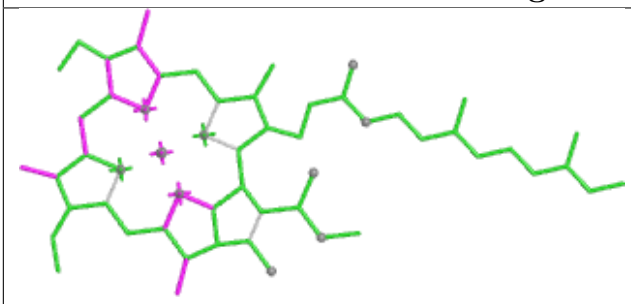


Torsions

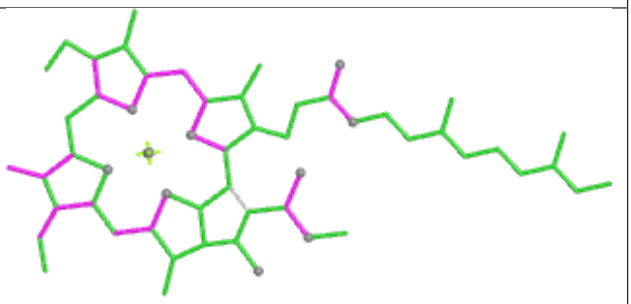


Rings

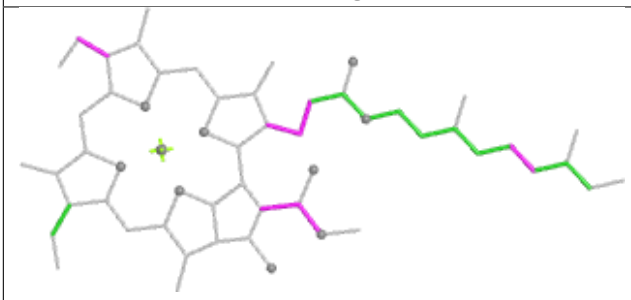
Ligand CLA 5 610



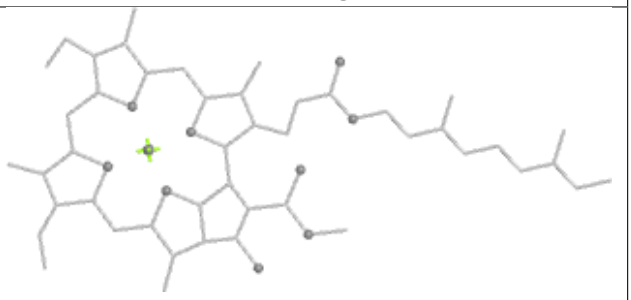
Bond lengths



Bond angles

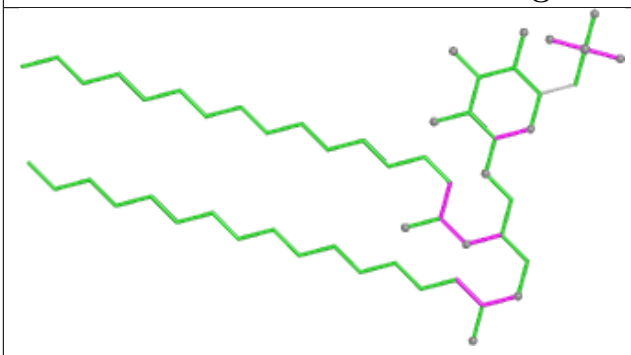


Torsions

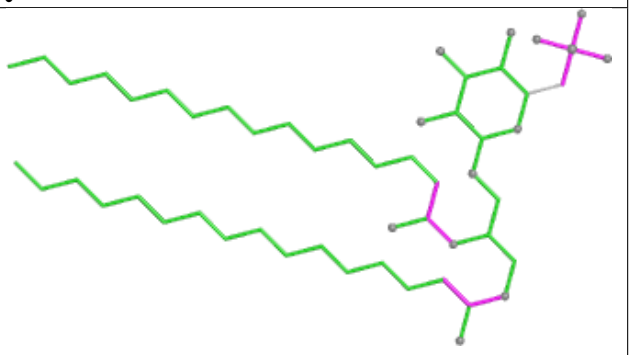


Rings

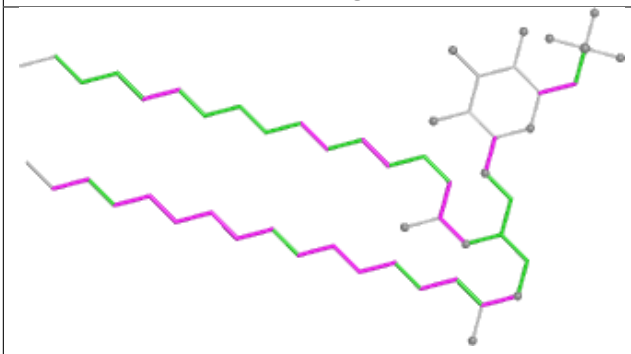
Ligand SQD l 101



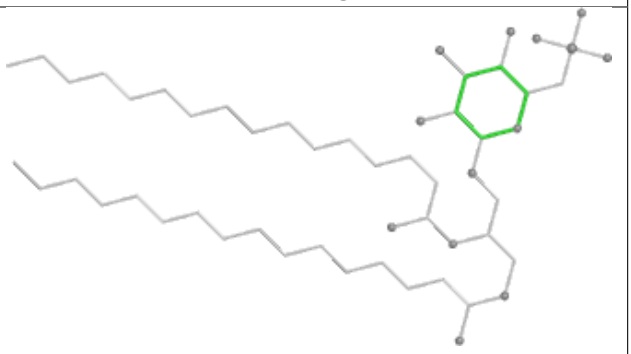
Bond lengths



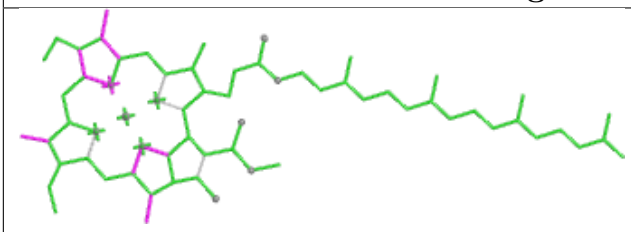
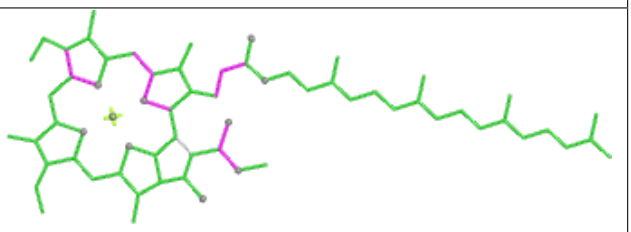
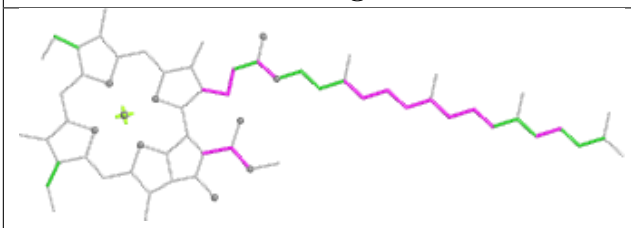
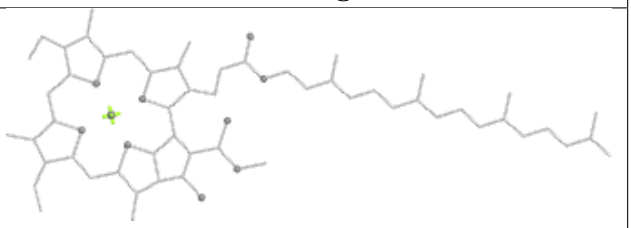
Bond angles

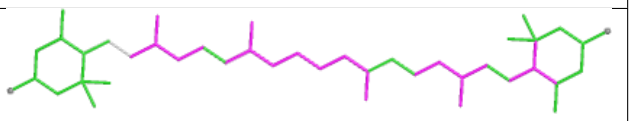
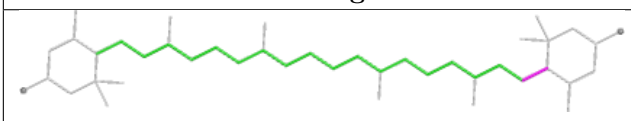
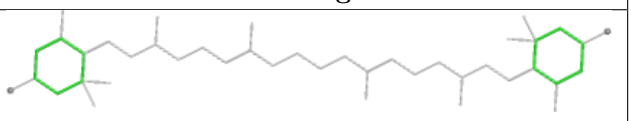


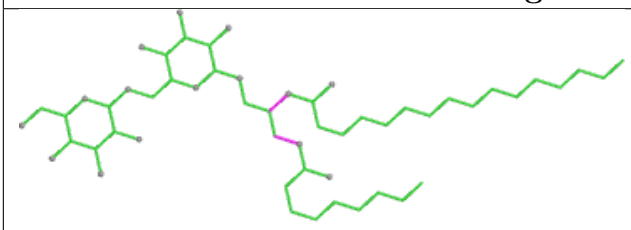
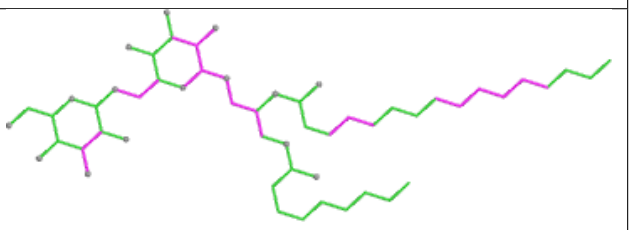
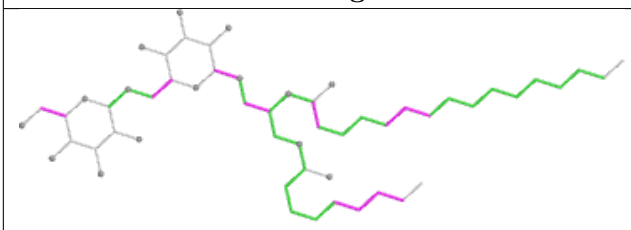
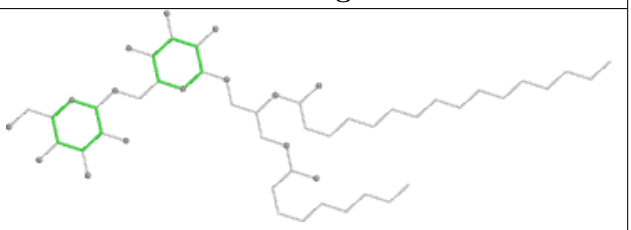
Torsions

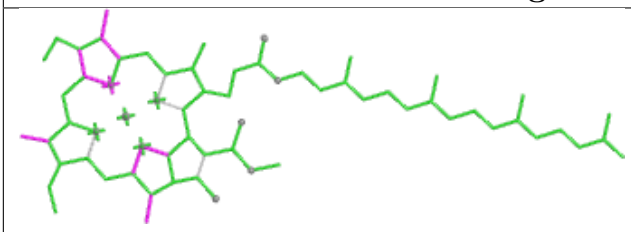
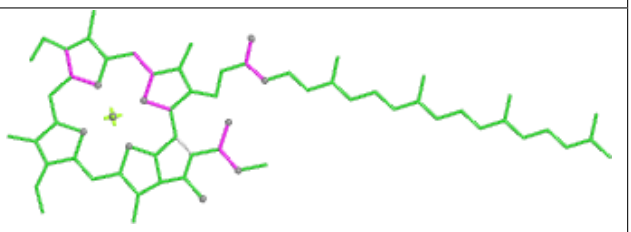
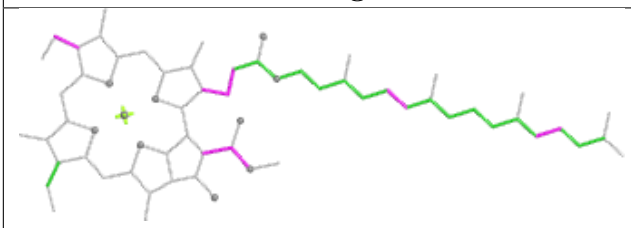
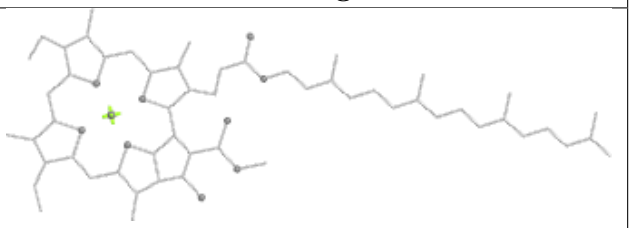


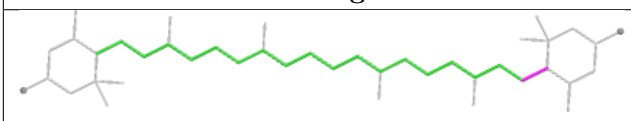
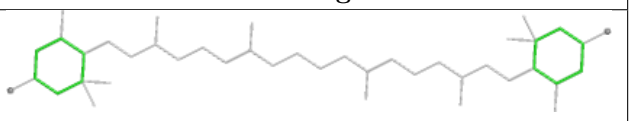
Rings

Ligand CLA b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT A6 615	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD c 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT Au 615	
Bond lengths	Bond angles
 Torsions	 Rings

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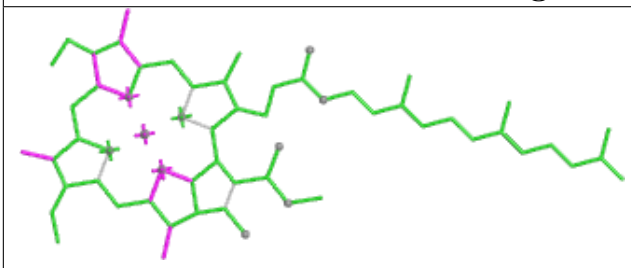
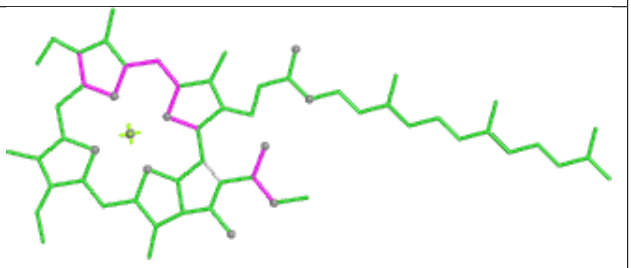
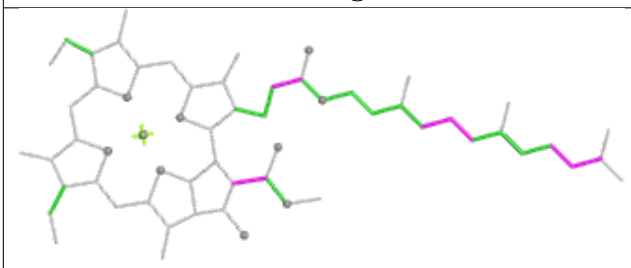
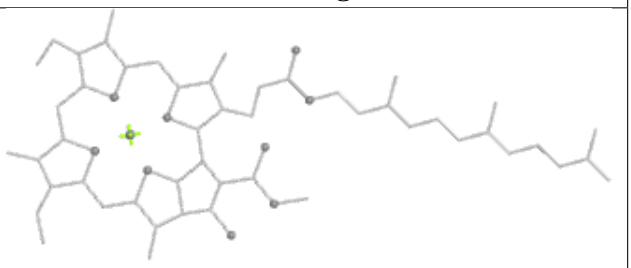
 Bond lengths	 Bond angles
 Torsions	 Rings

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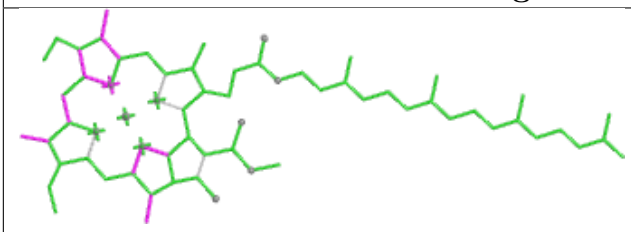
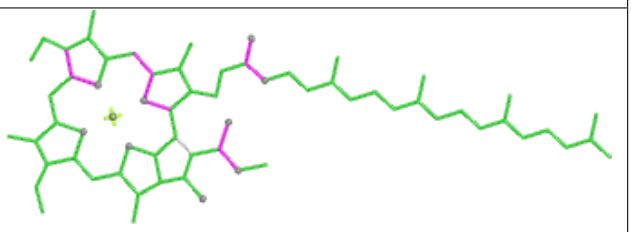
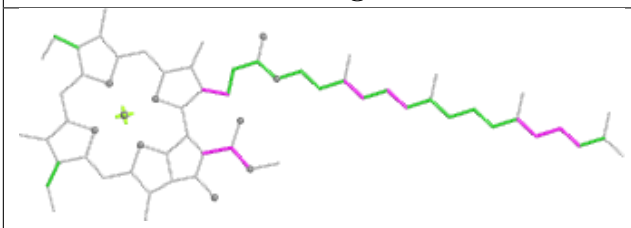
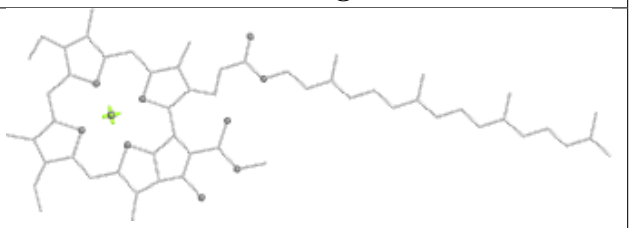
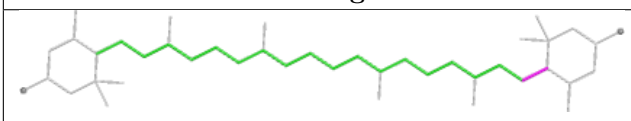
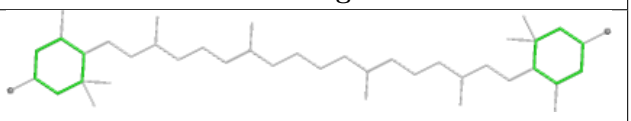
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT A2 615	
Bond lengths	Bond angles
 Torsions	 Rings

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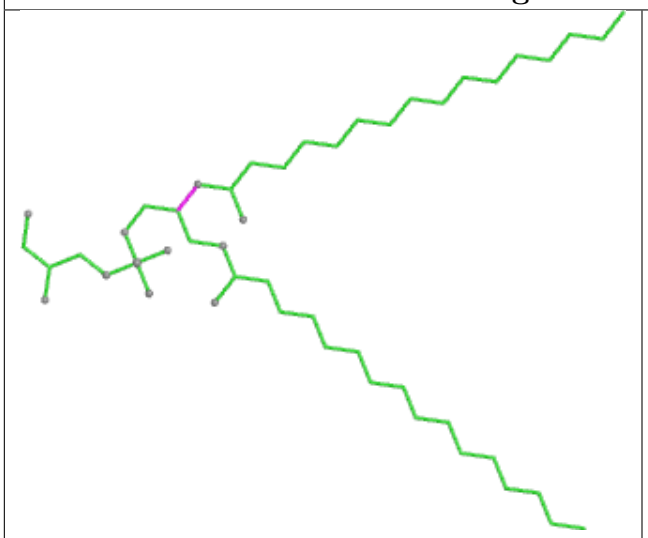
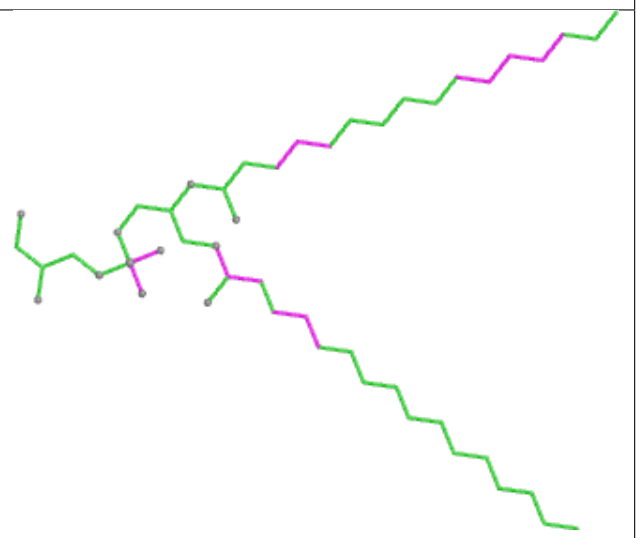
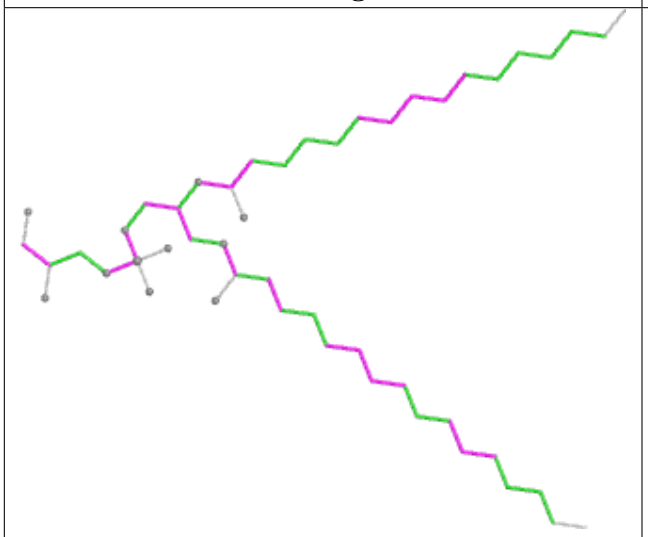


Bond lengths



Bond angles



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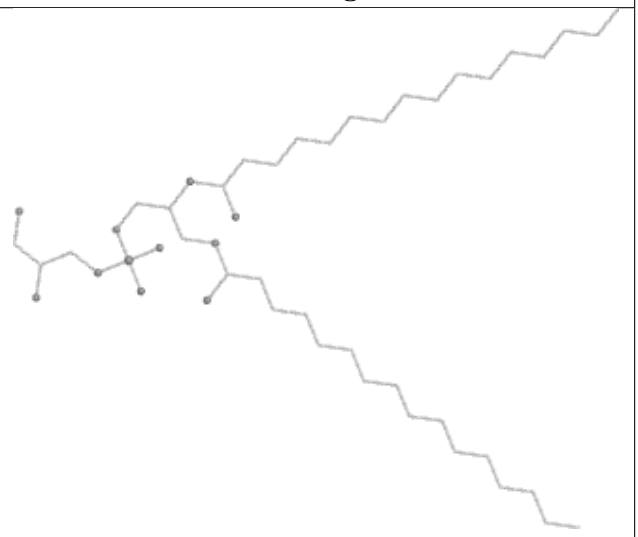
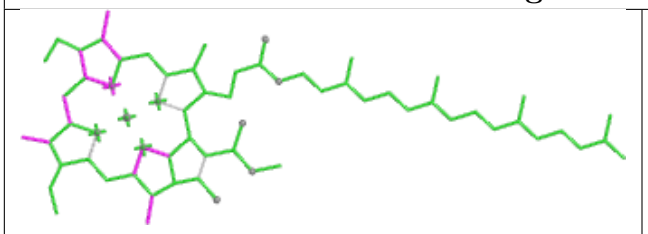
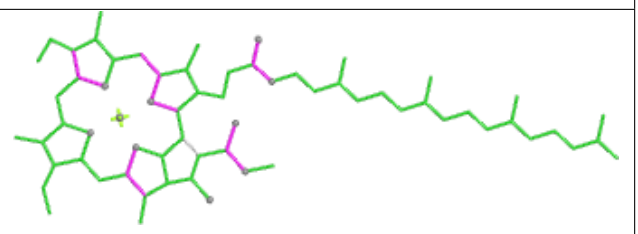


Rings

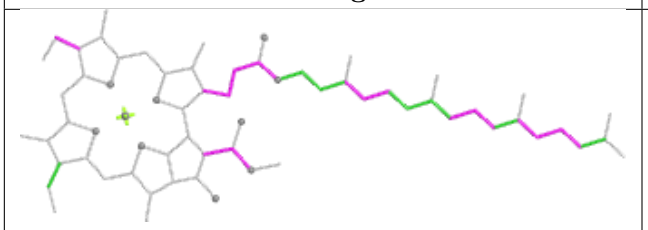
Ligand CLA B 605



Bond lengths



Bond angles



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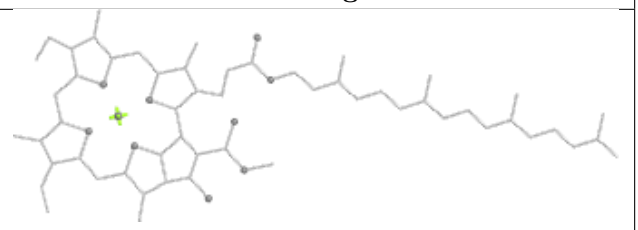
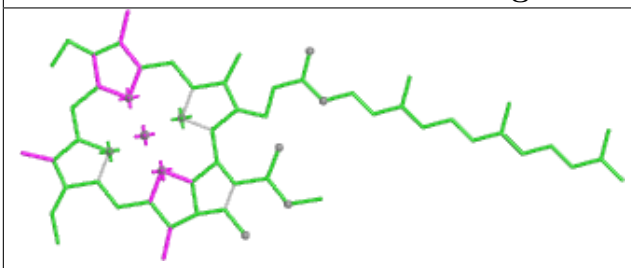
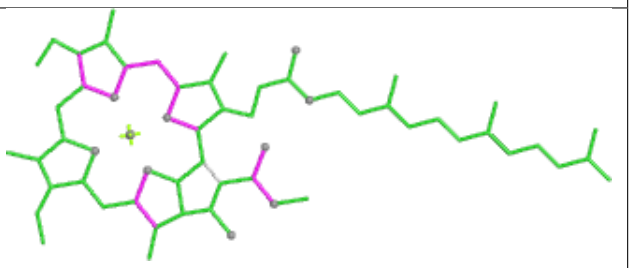
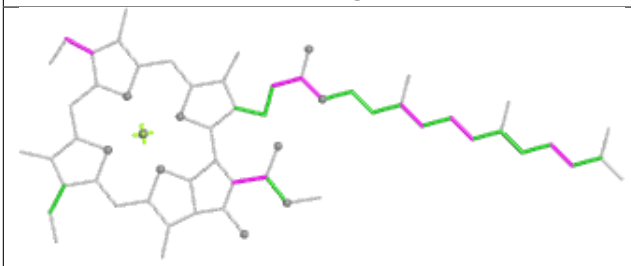
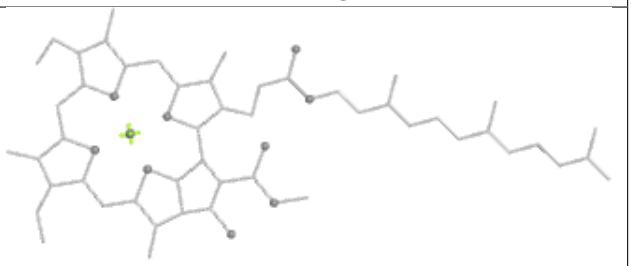
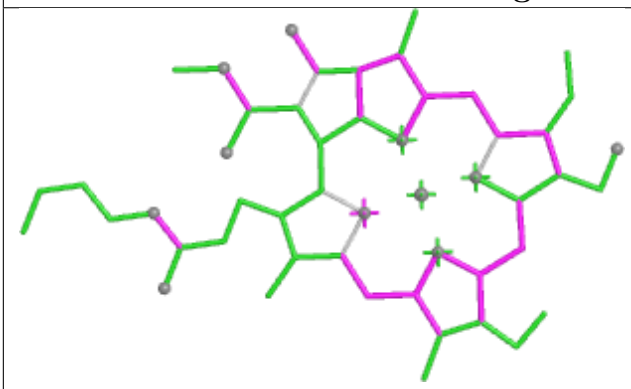
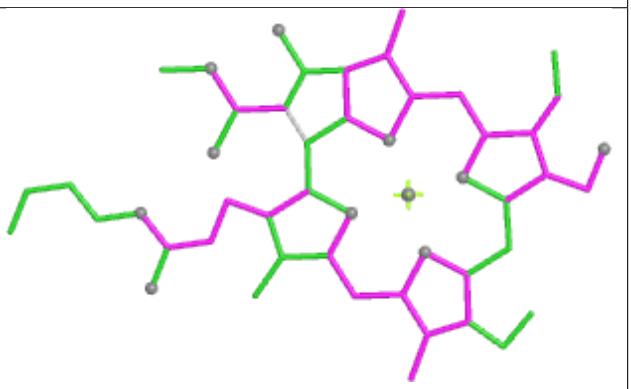
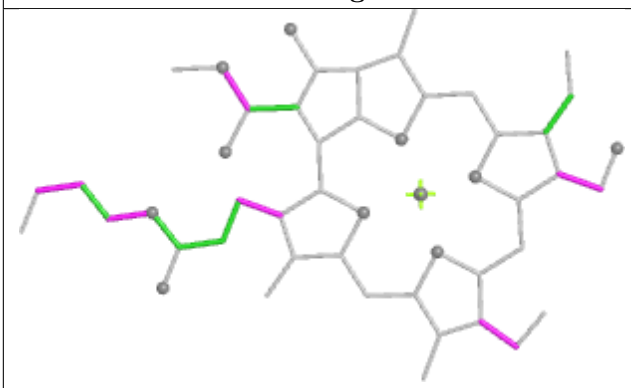
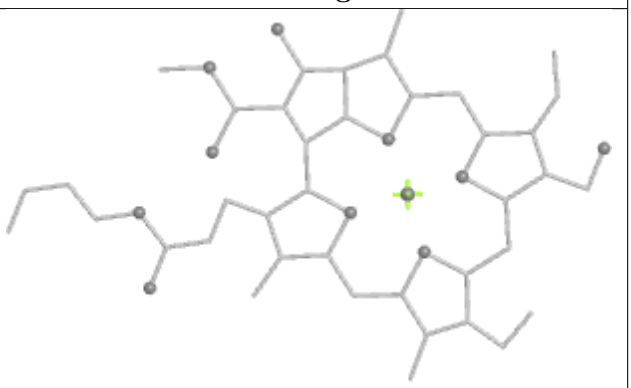
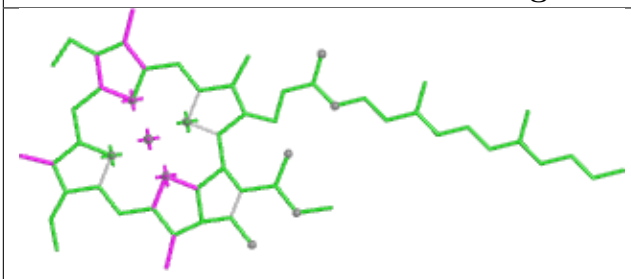


Rings

Ligand CLA BB 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Au 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 608



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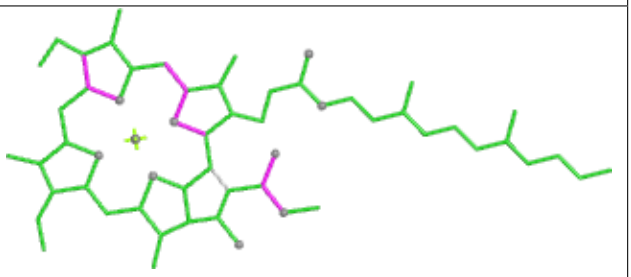
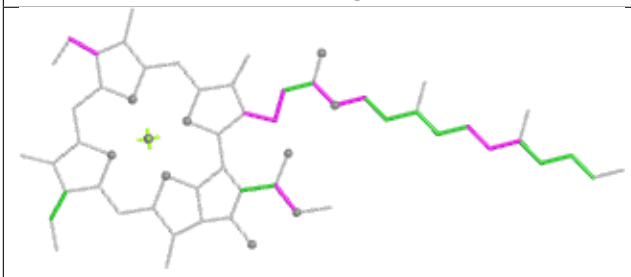
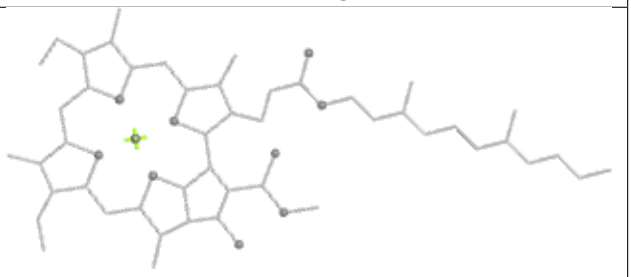


Bond angles

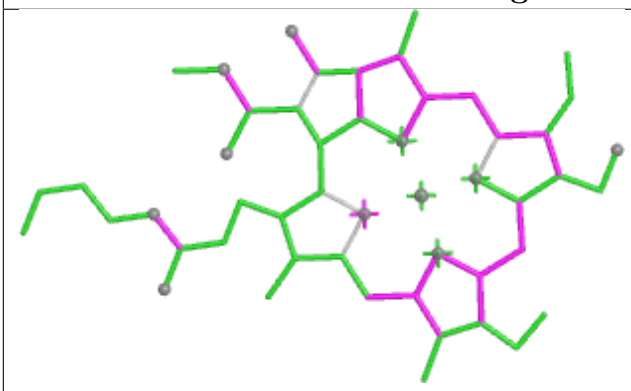


Torsions



Rings

Ligand CHL BQ 606



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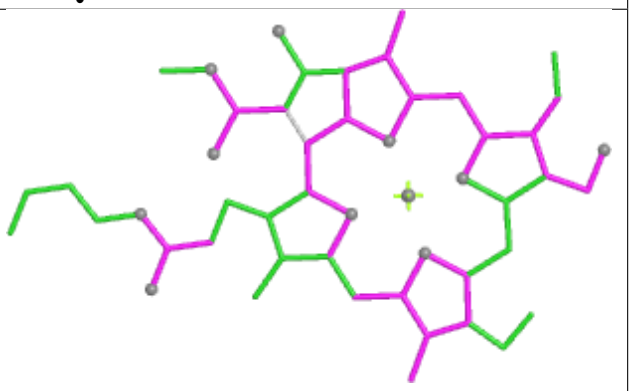
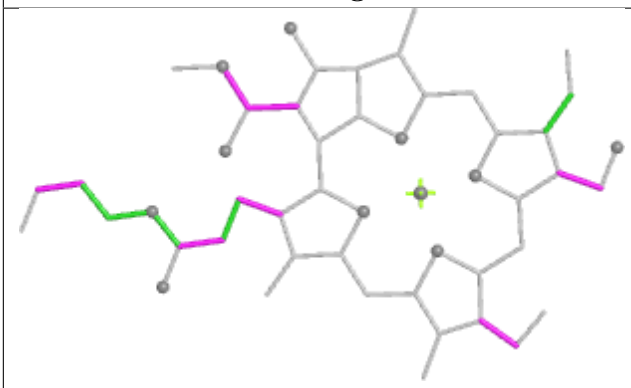


Bond angles



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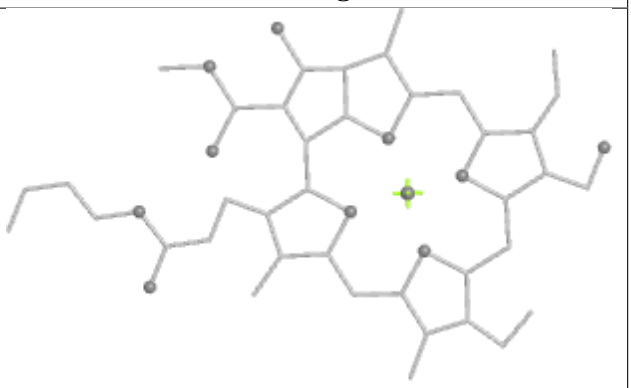
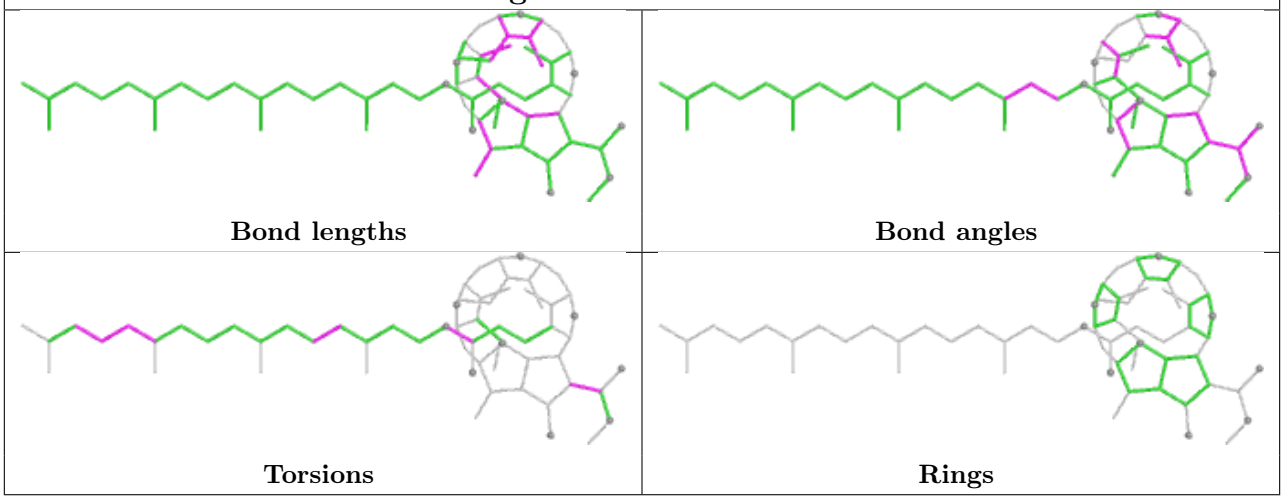


Rings

Ligand PHO BD 408



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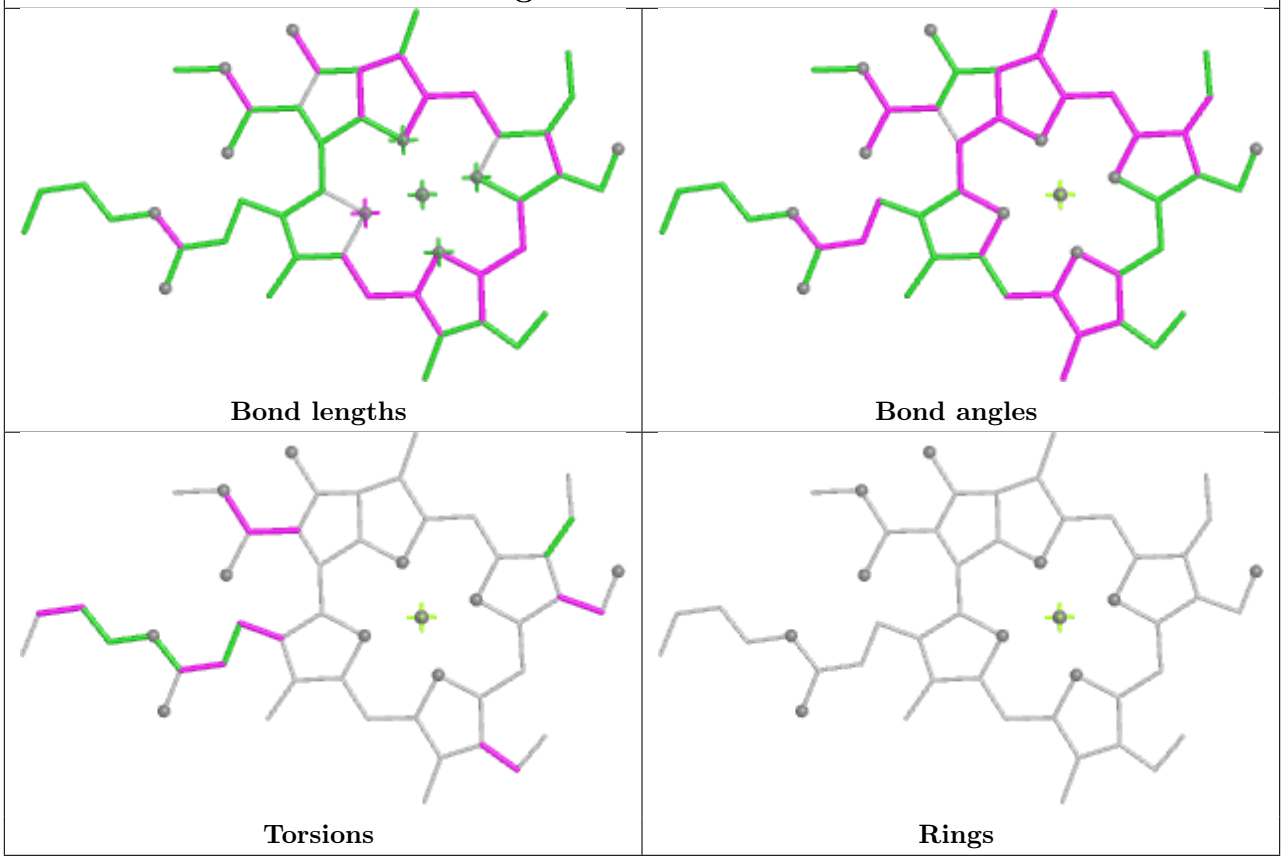

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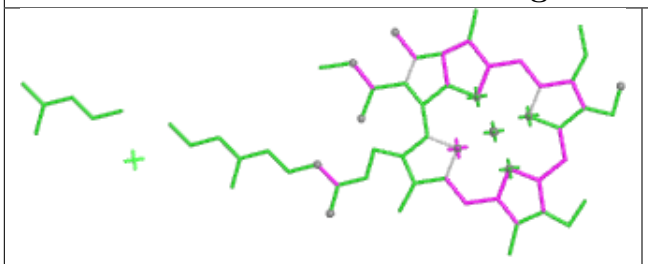

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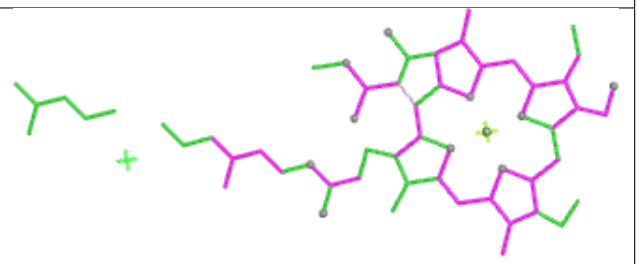
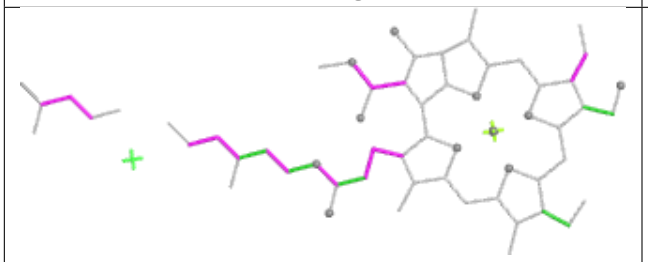


Bond angles



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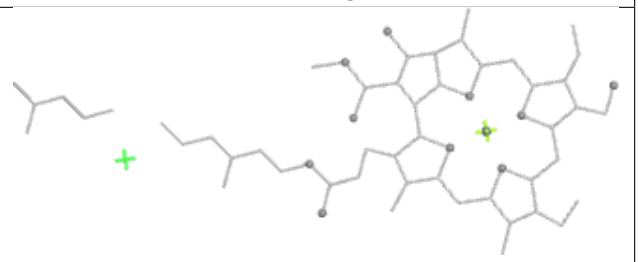
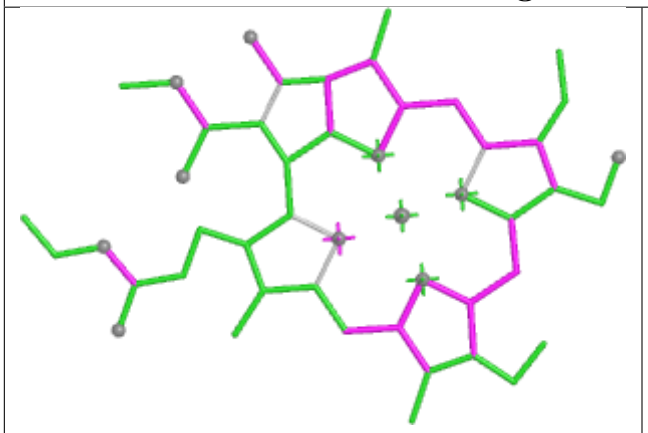
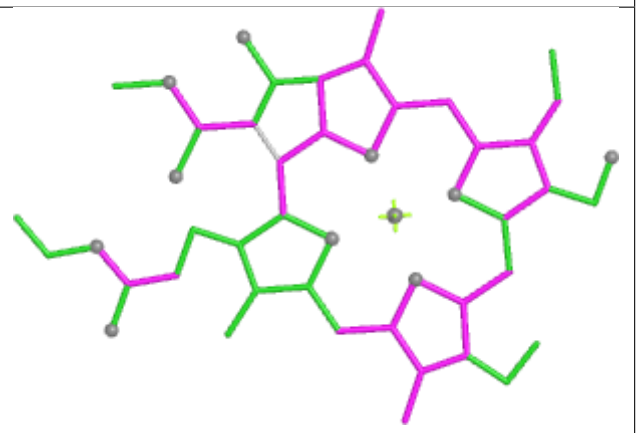


Rings

Ligand CHL Ba 306



Bond lengths



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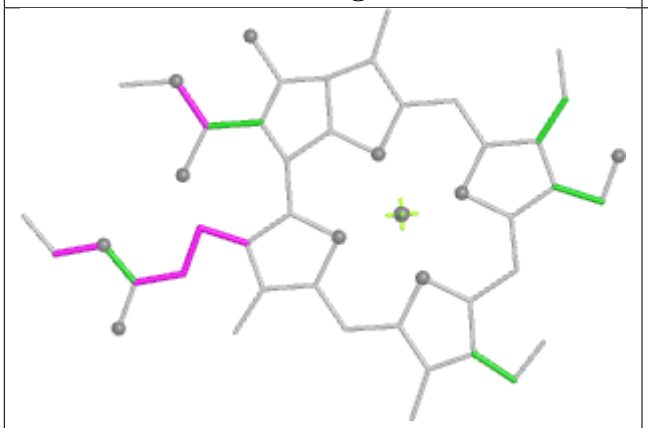

Torsions

Rings

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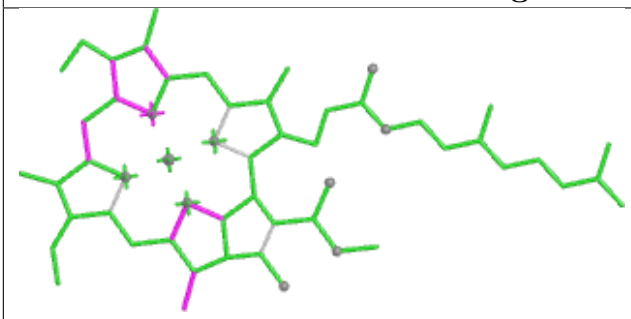
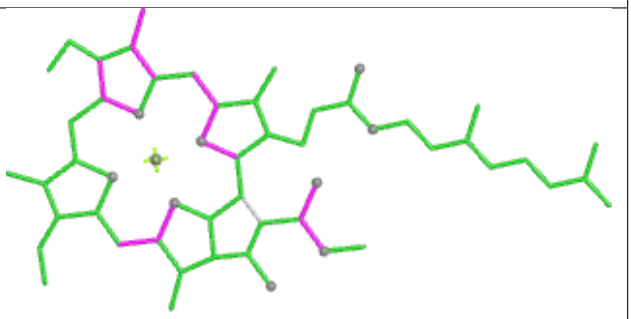
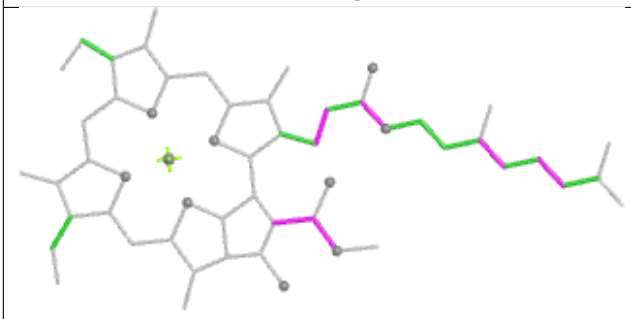
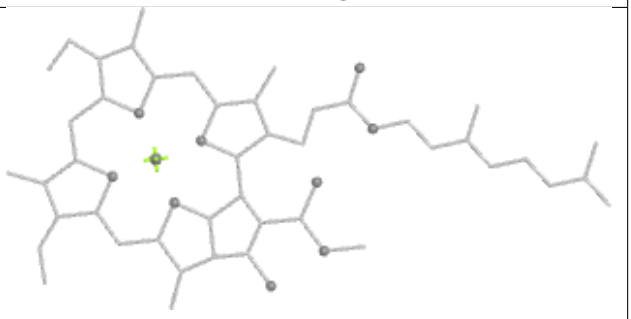
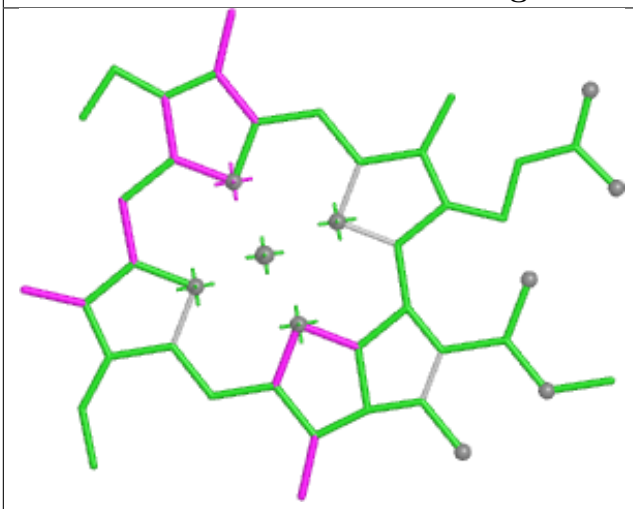
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 305



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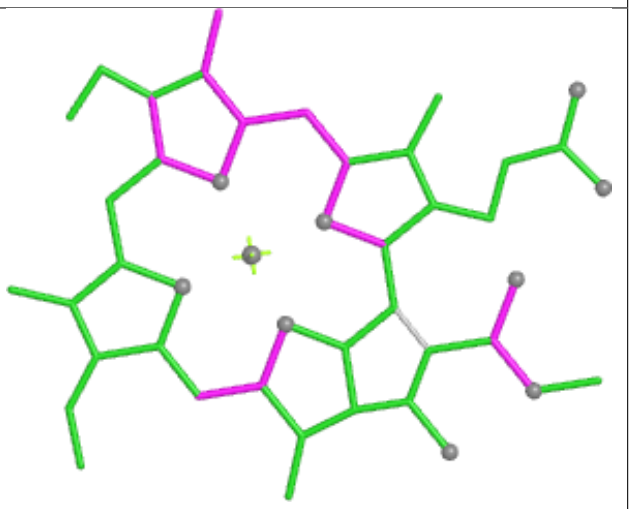

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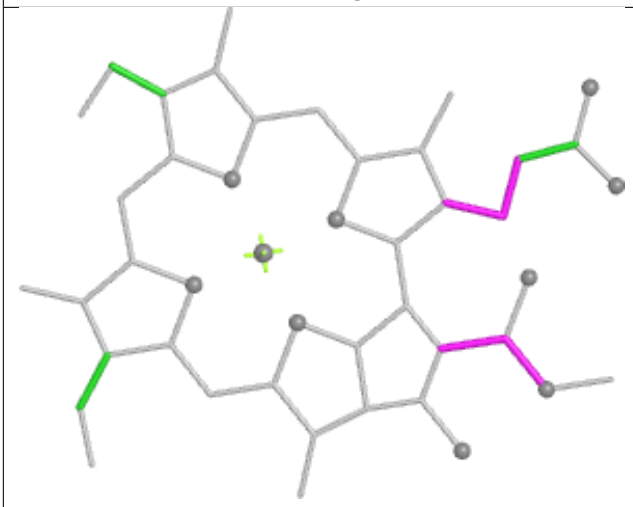
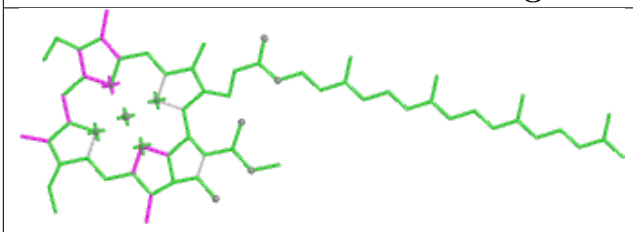


Torsions

Rings

Ligand CLA B 607



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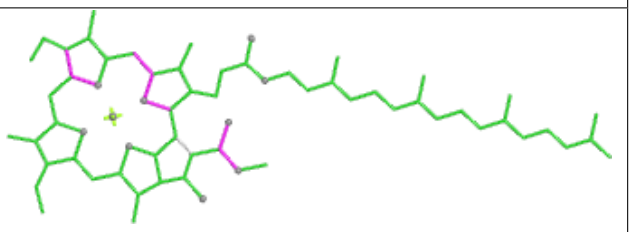

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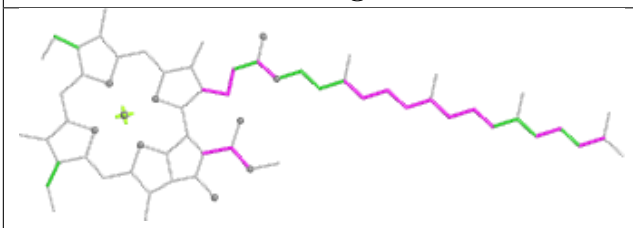

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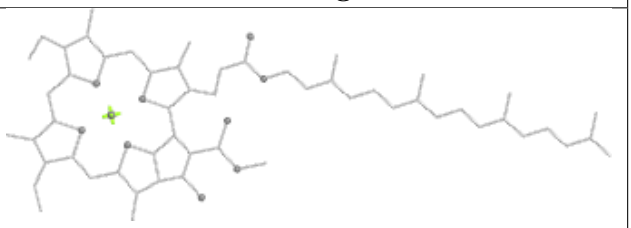
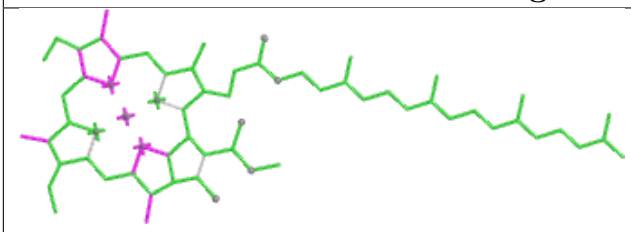
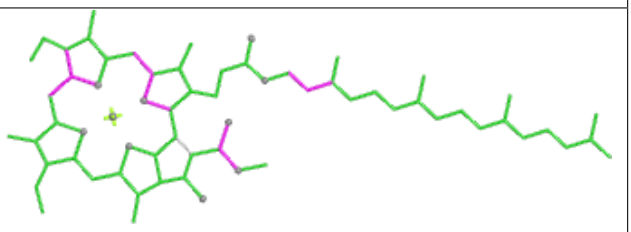
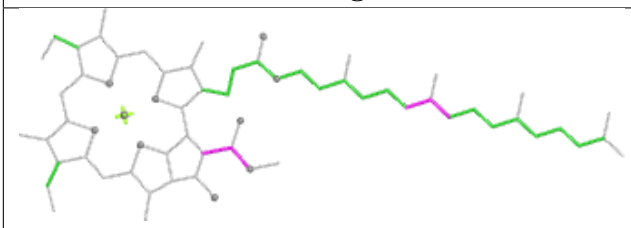
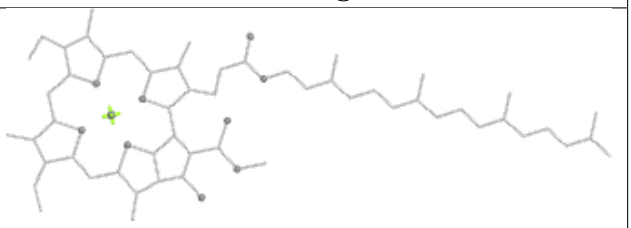
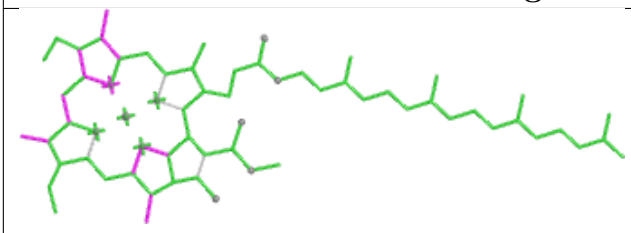
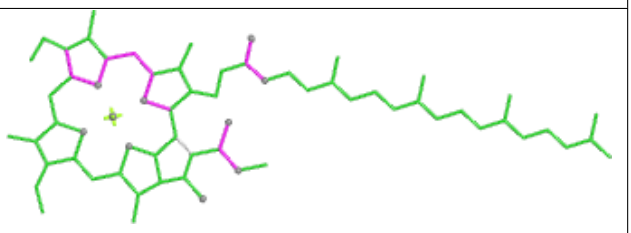
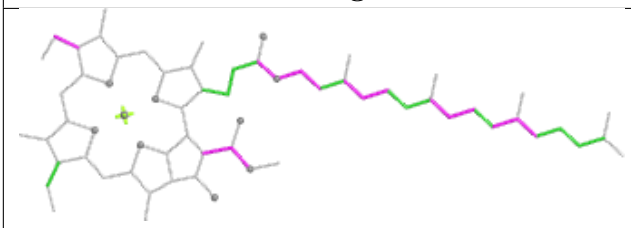
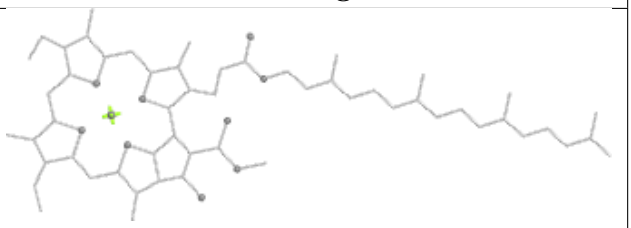


Rings

Ligand CLA c 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

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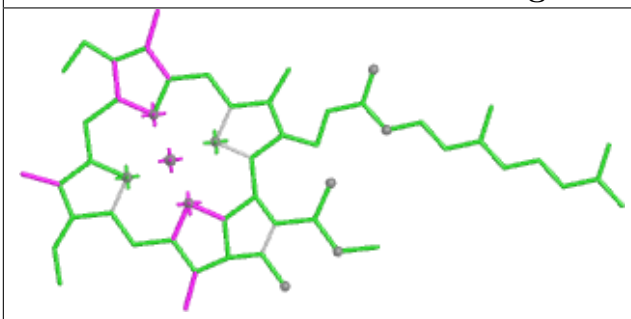
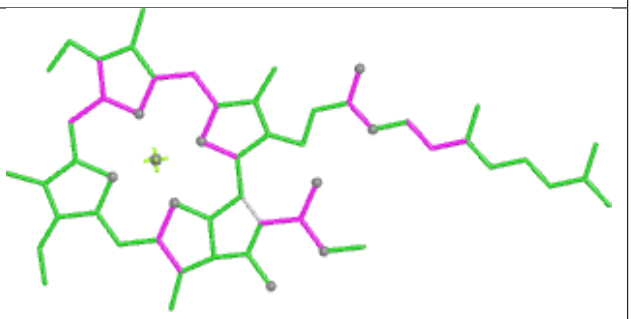
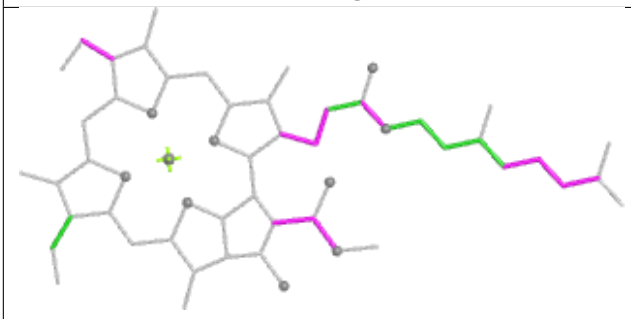
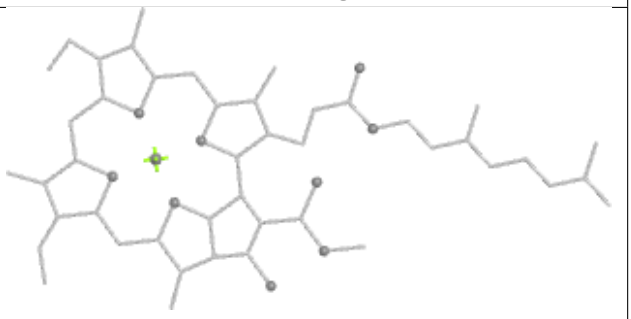
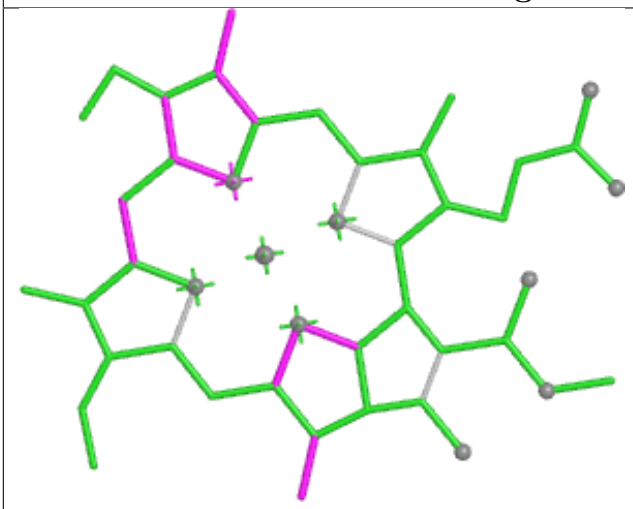
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A6 608



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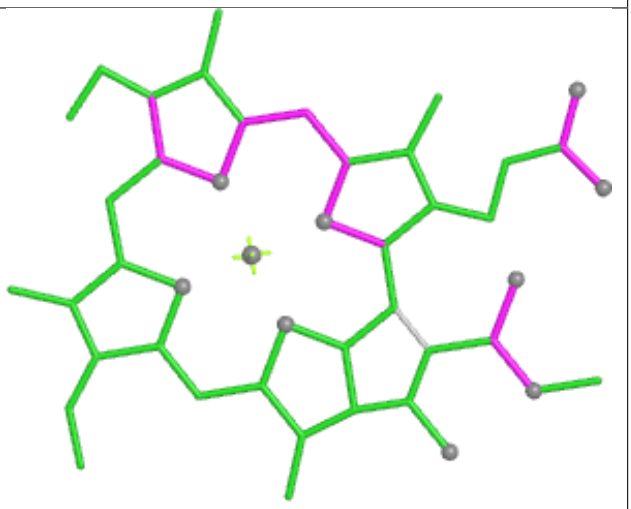
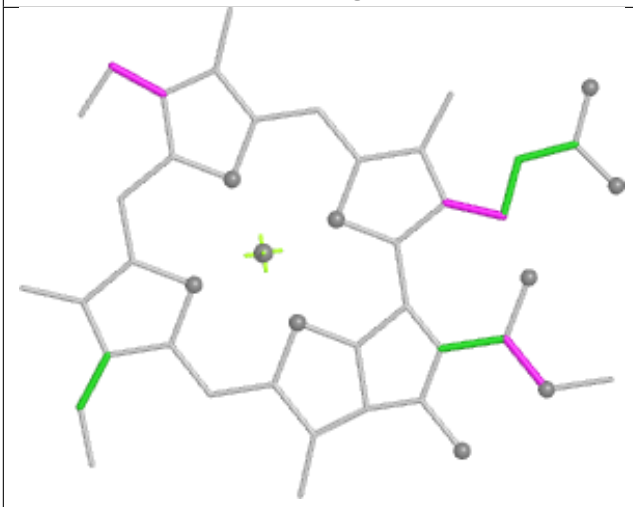


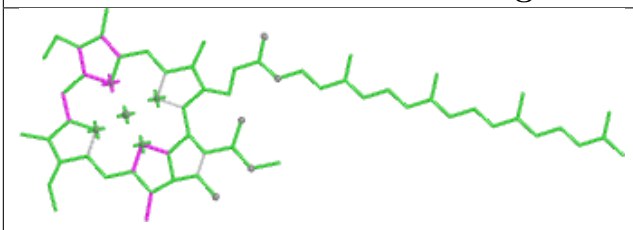
Bond angles



Torsions

Rings

Ligand CLA BJ 603



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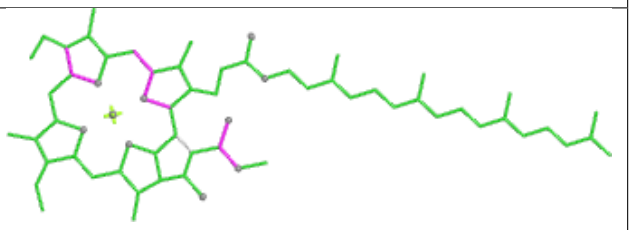
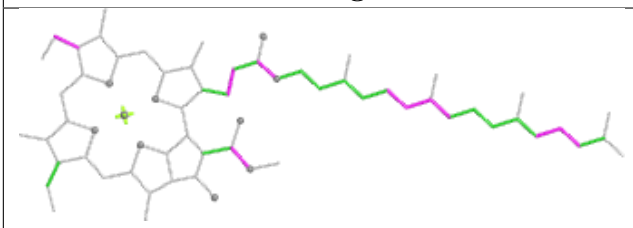


Bond angles



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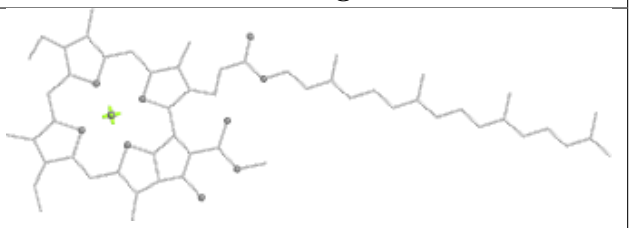
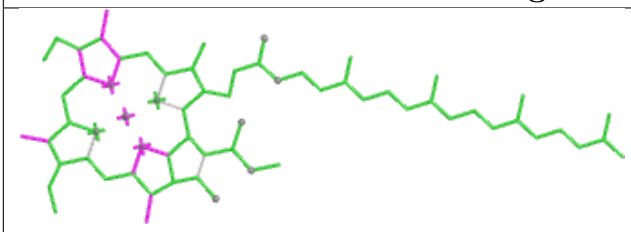
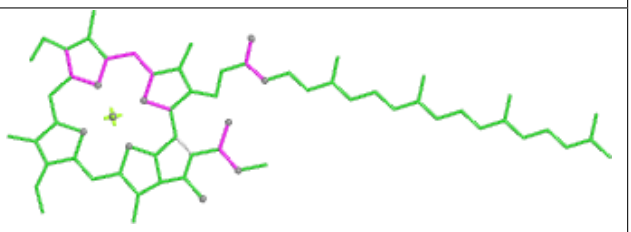
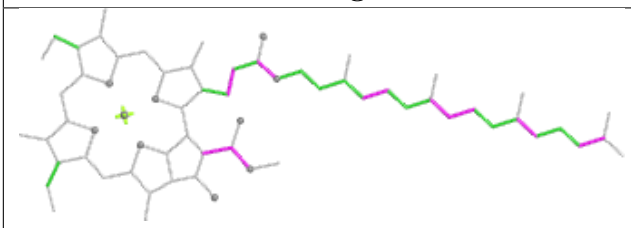
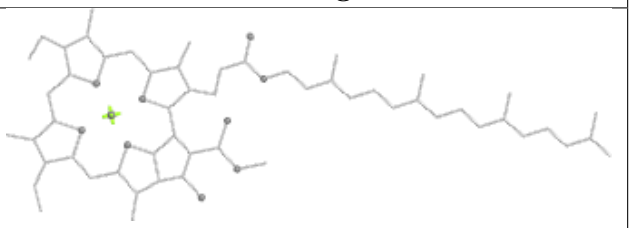
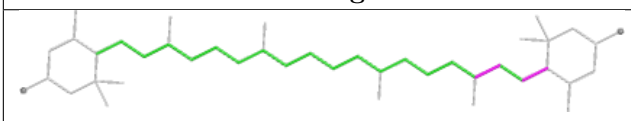
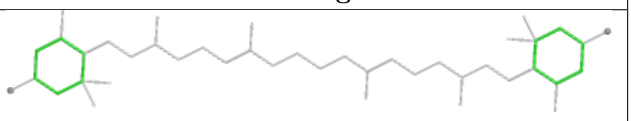


Rings

Ligand CLA 1 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 9 615	
Bond lengths	Bond angles
 Torsions	 Rings

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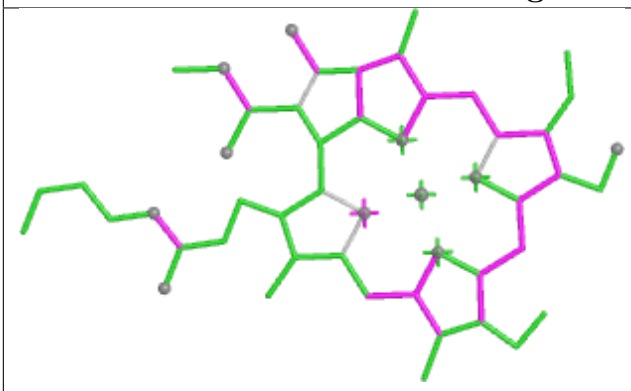
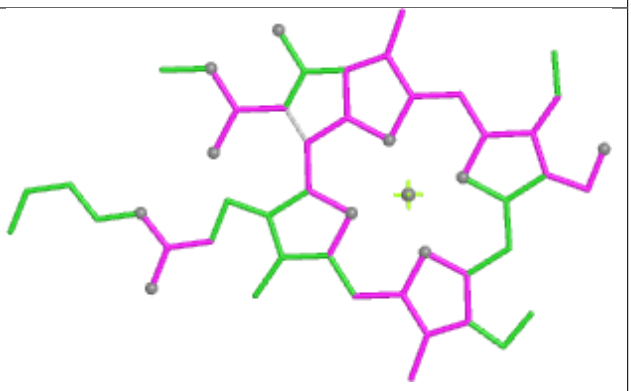
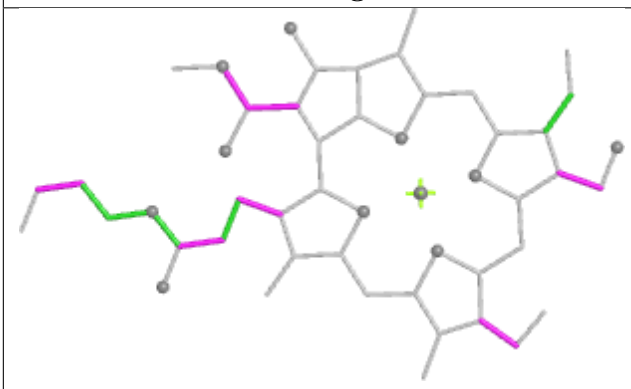
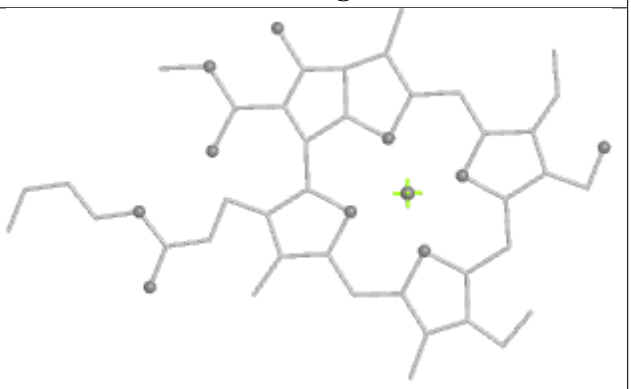
 Bond lengths	 Bond angles
 Torsions	 Rings

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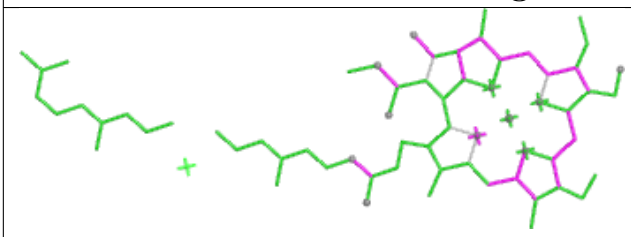
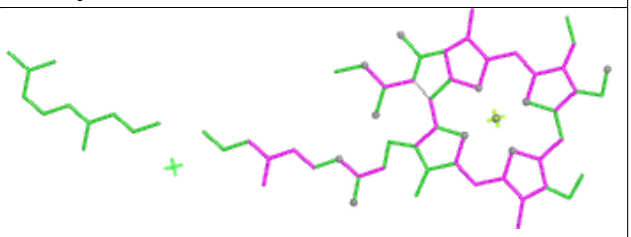
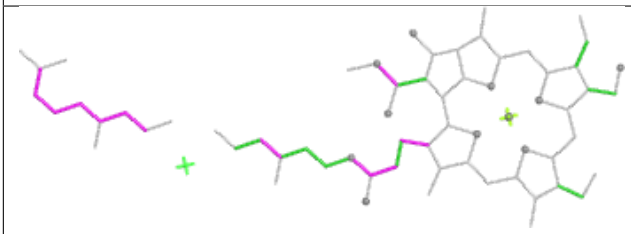
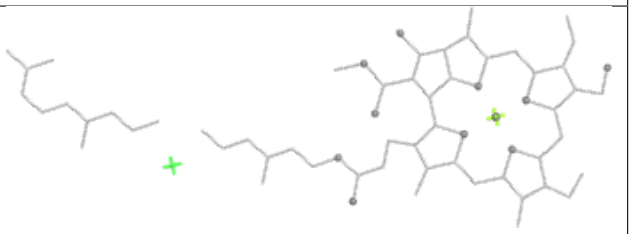
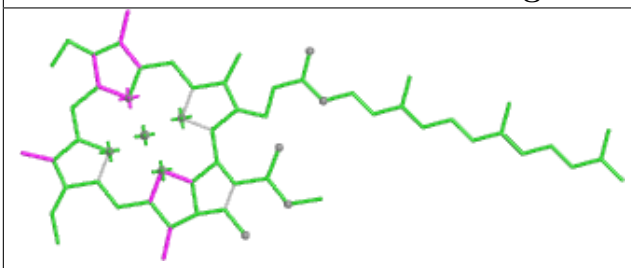
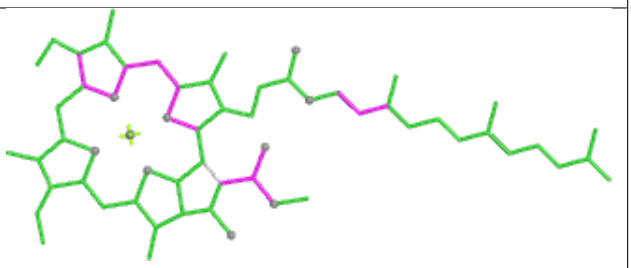
 Bond lengths	 Bond angles
 Torsions	 Rings

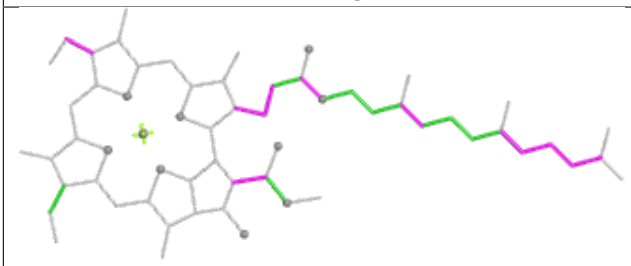
Ligand CLA N 611



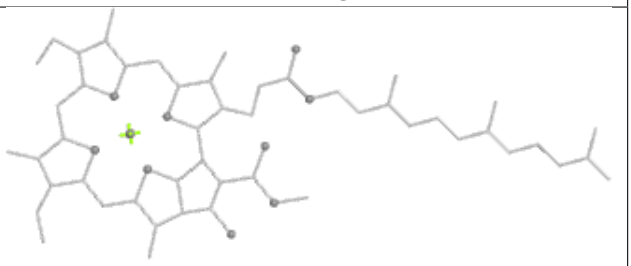
Bond lengths



Bond angles

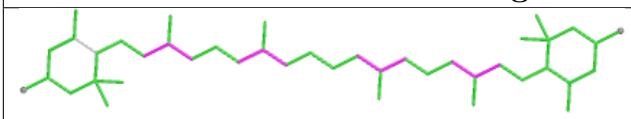


Torsions



Rings

Ligand LUT BU 615



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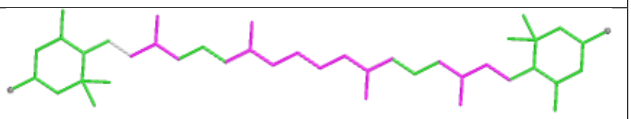
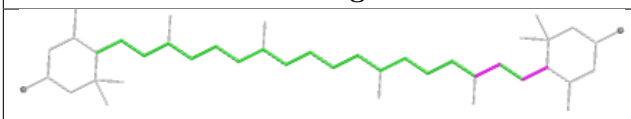
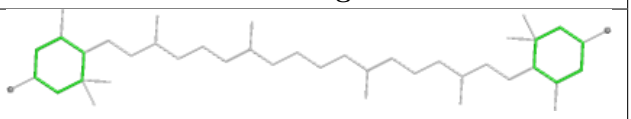


Bond angles

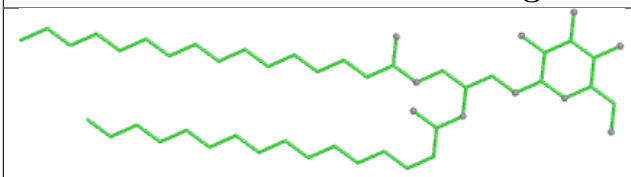


Torsions

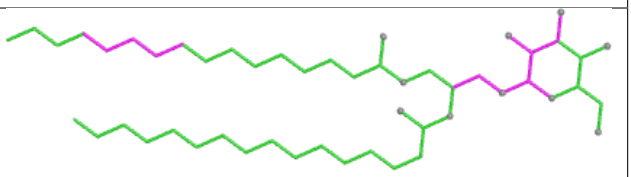


Rings

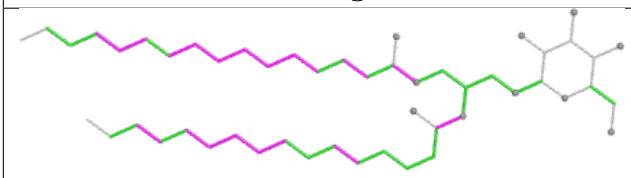
Ligand LMG v 620



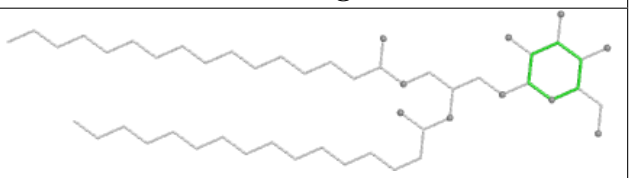
Bond lengths



Bond angles

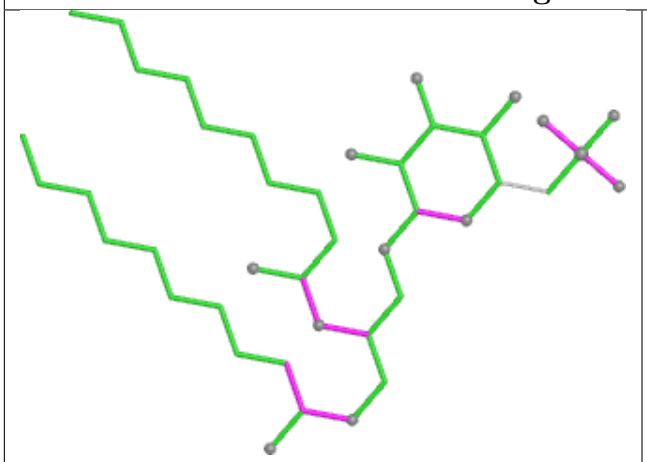


Torsions

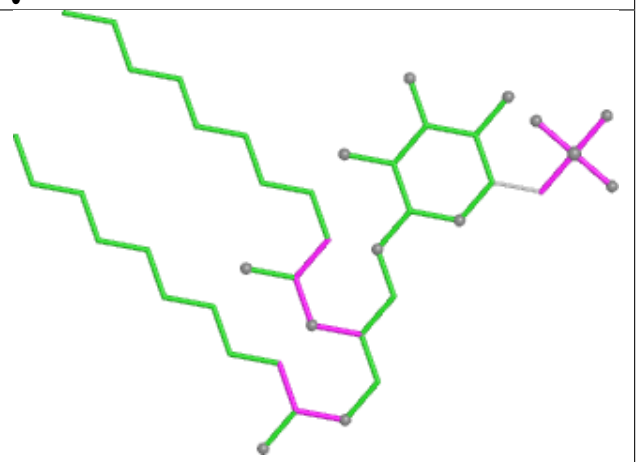


Rings

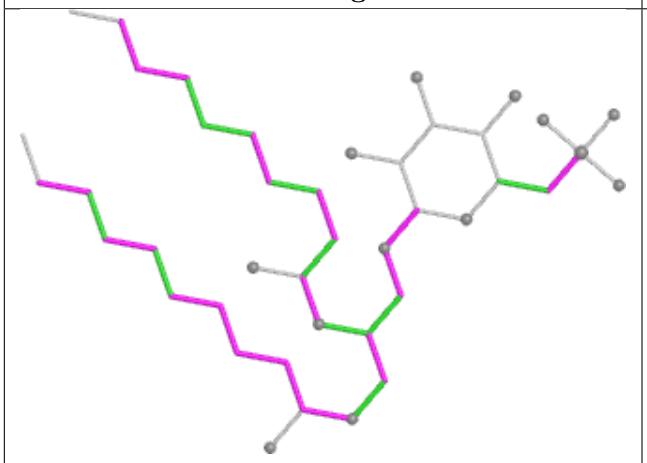
Ligand SQD l 102



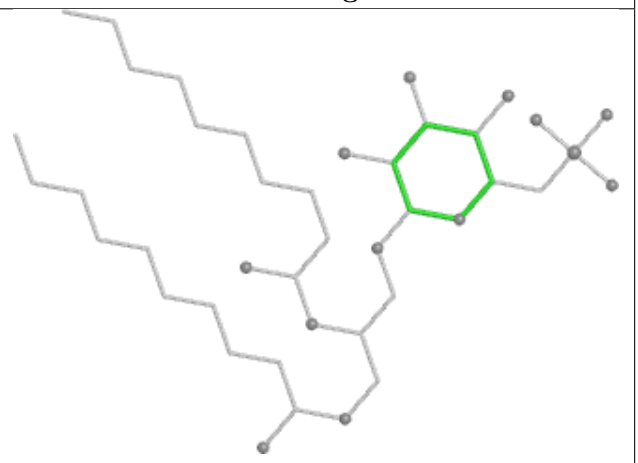
Bond lengths



Bond angles

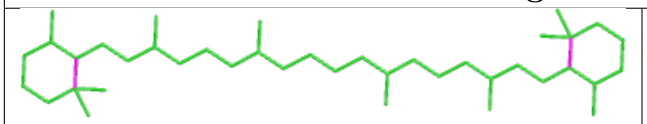


Torsions



Rings

Ligand BCR h 101



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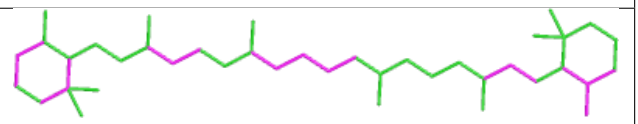

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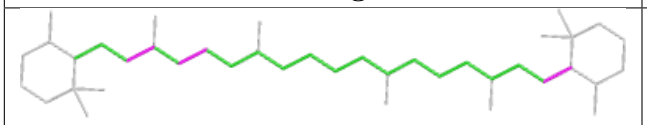

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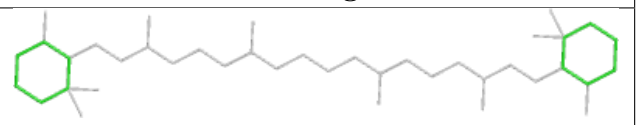
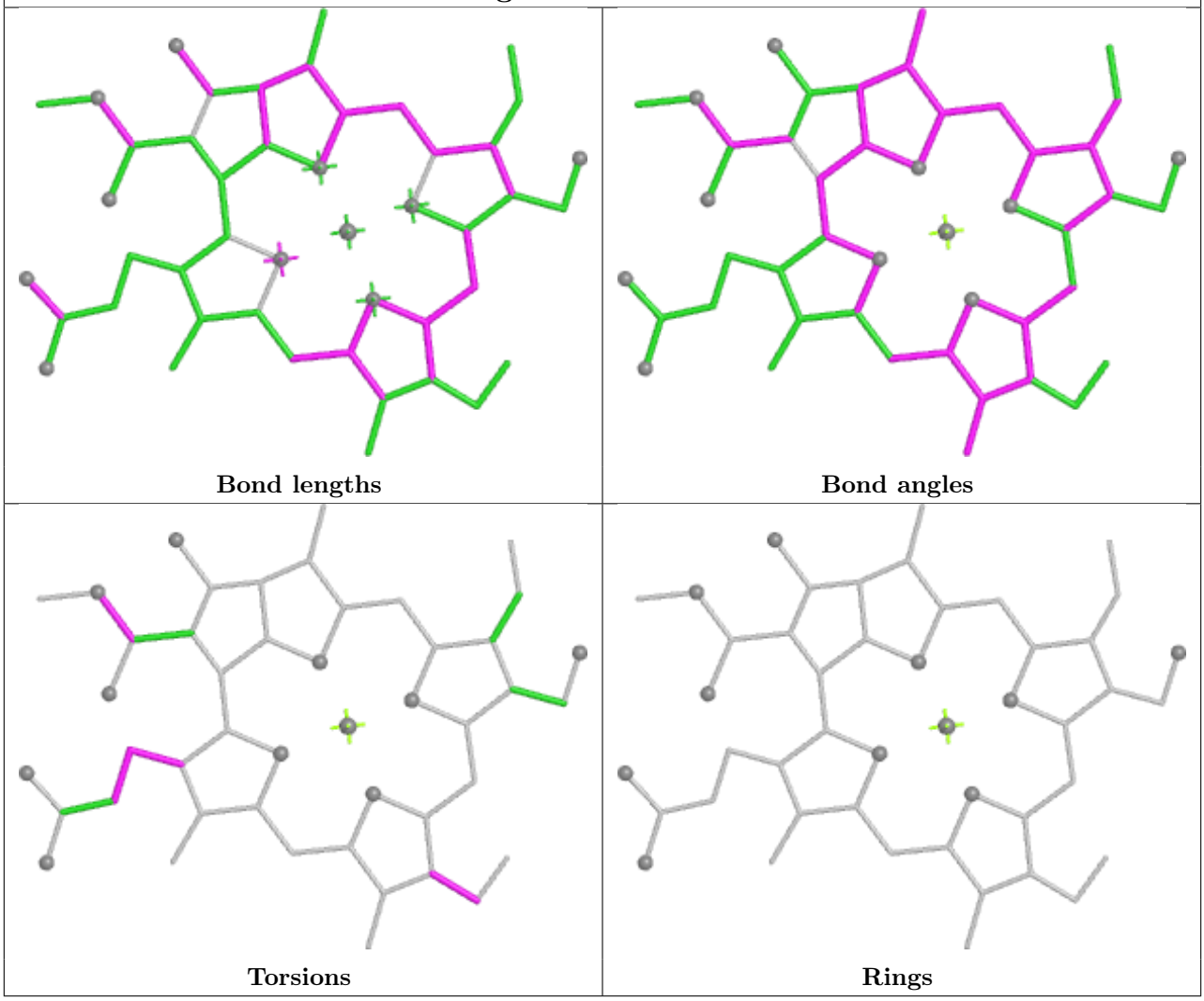


Rings

Ligand CHL 9 605



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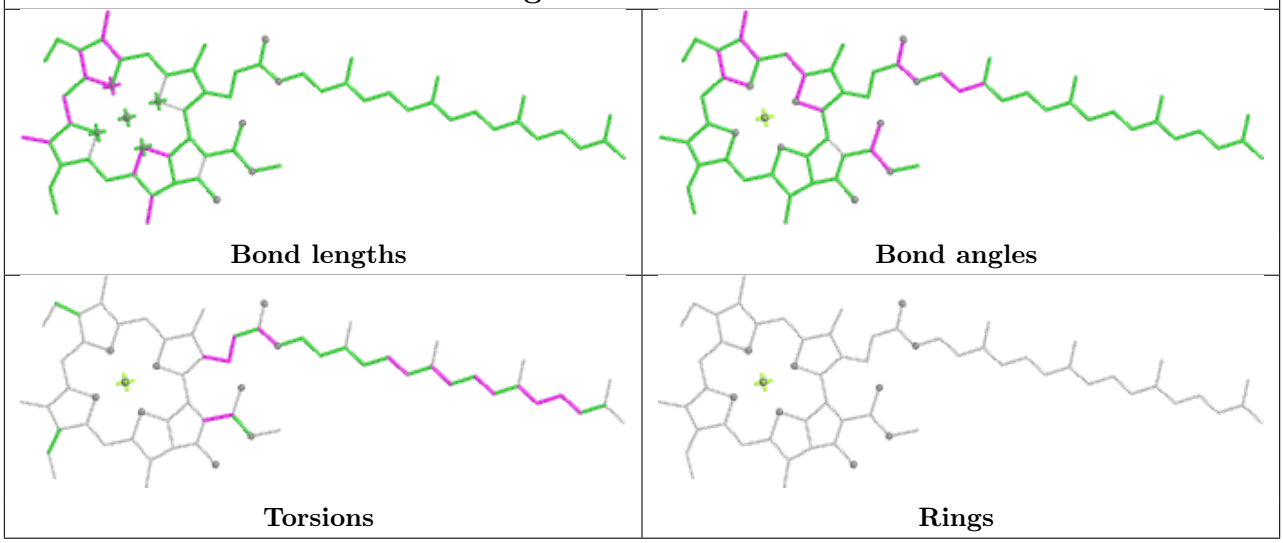

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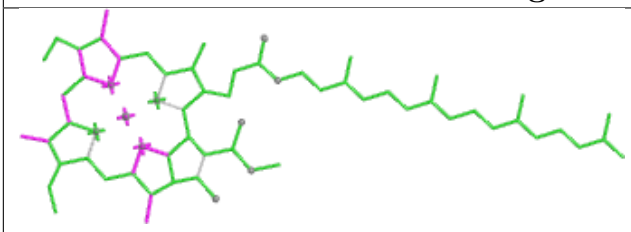
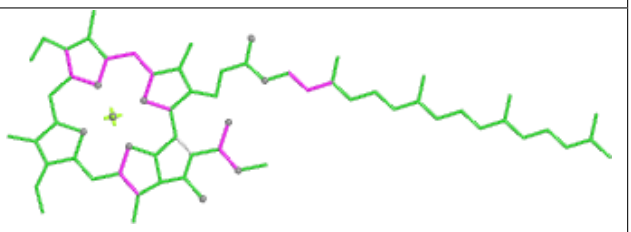
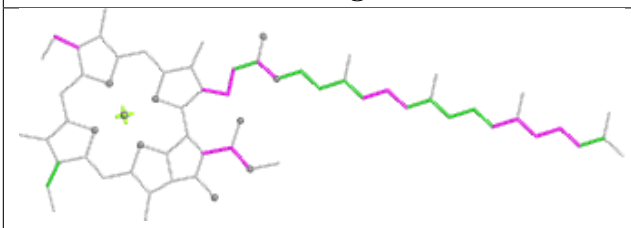
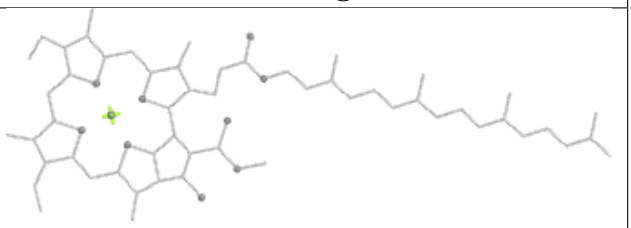
 Bond lengths	 Bond angles
 Torsions	 Rings

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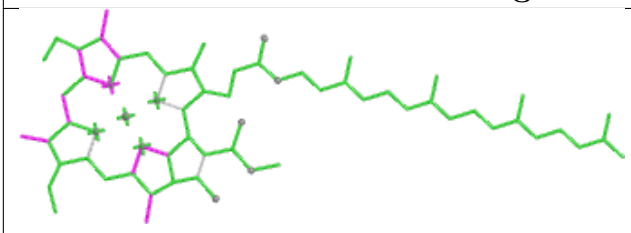
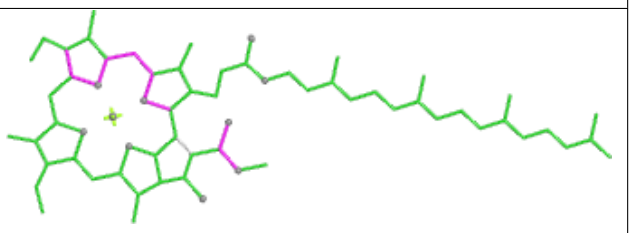
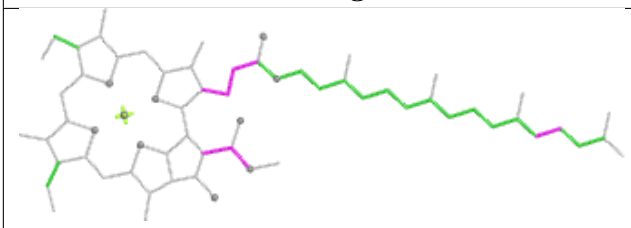
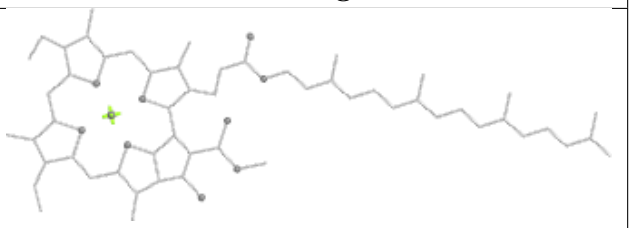
 Bond lengths	 Bond angles
 Torsions	 Rings

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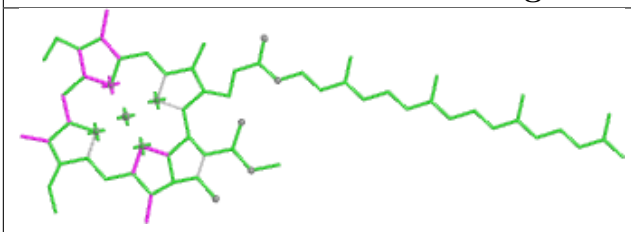
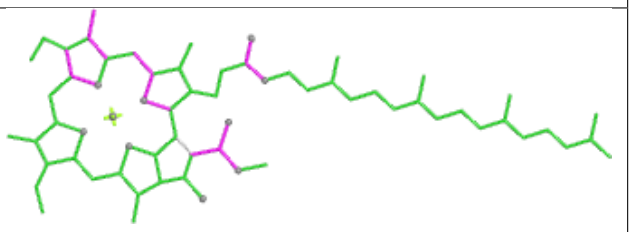
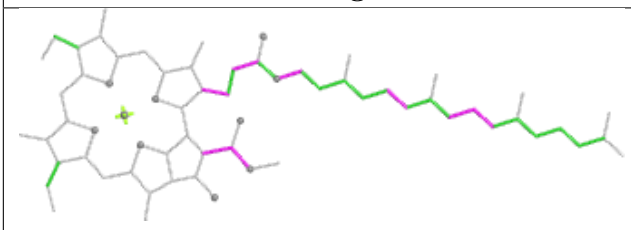
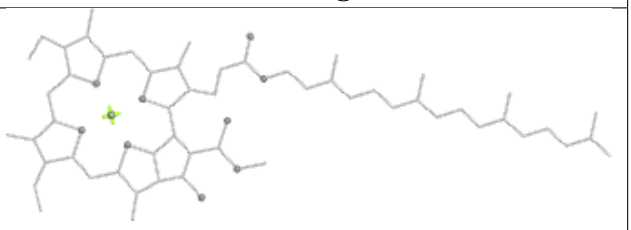
 Bond lengths	 Bond angles
 Torsions	 Rings

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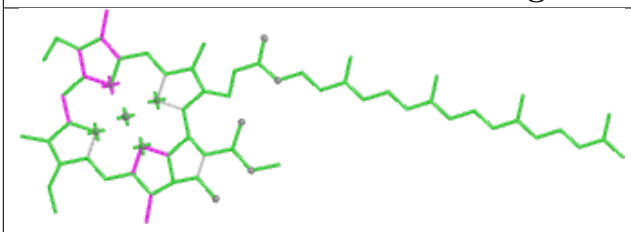
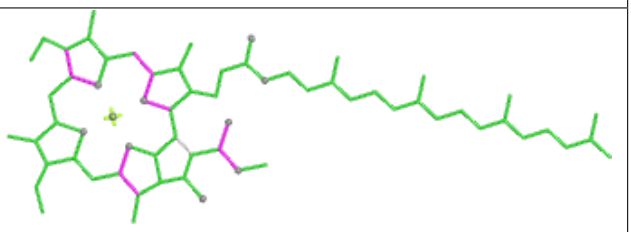
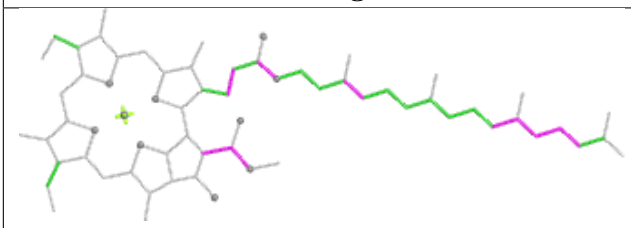
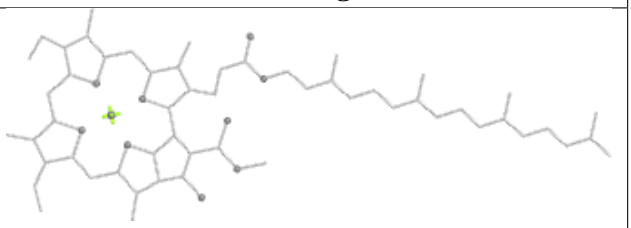
 Bond lengths	 Bond angles
 Torsions	 Rings

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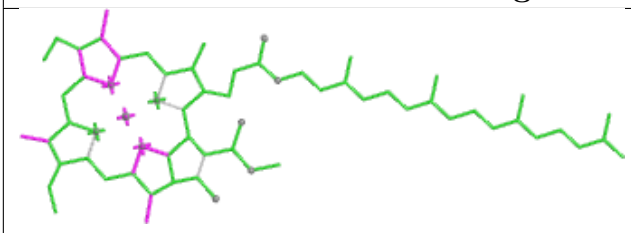
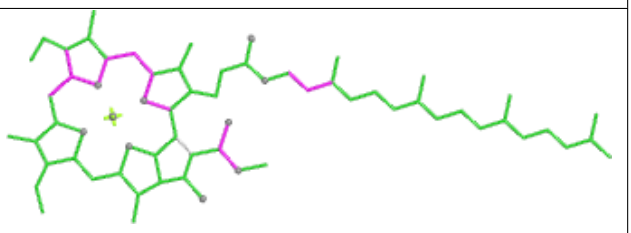
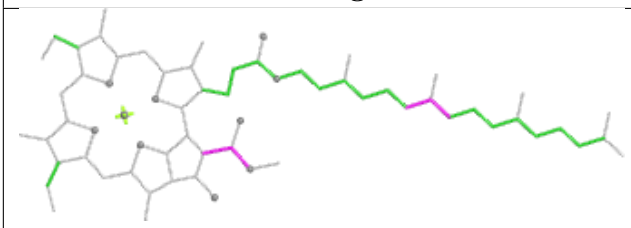
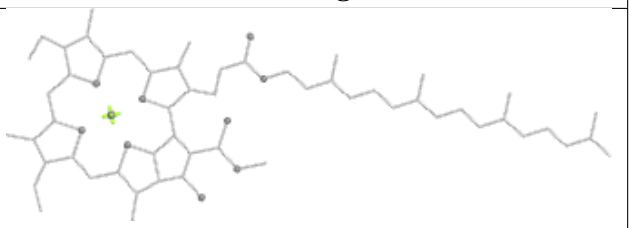
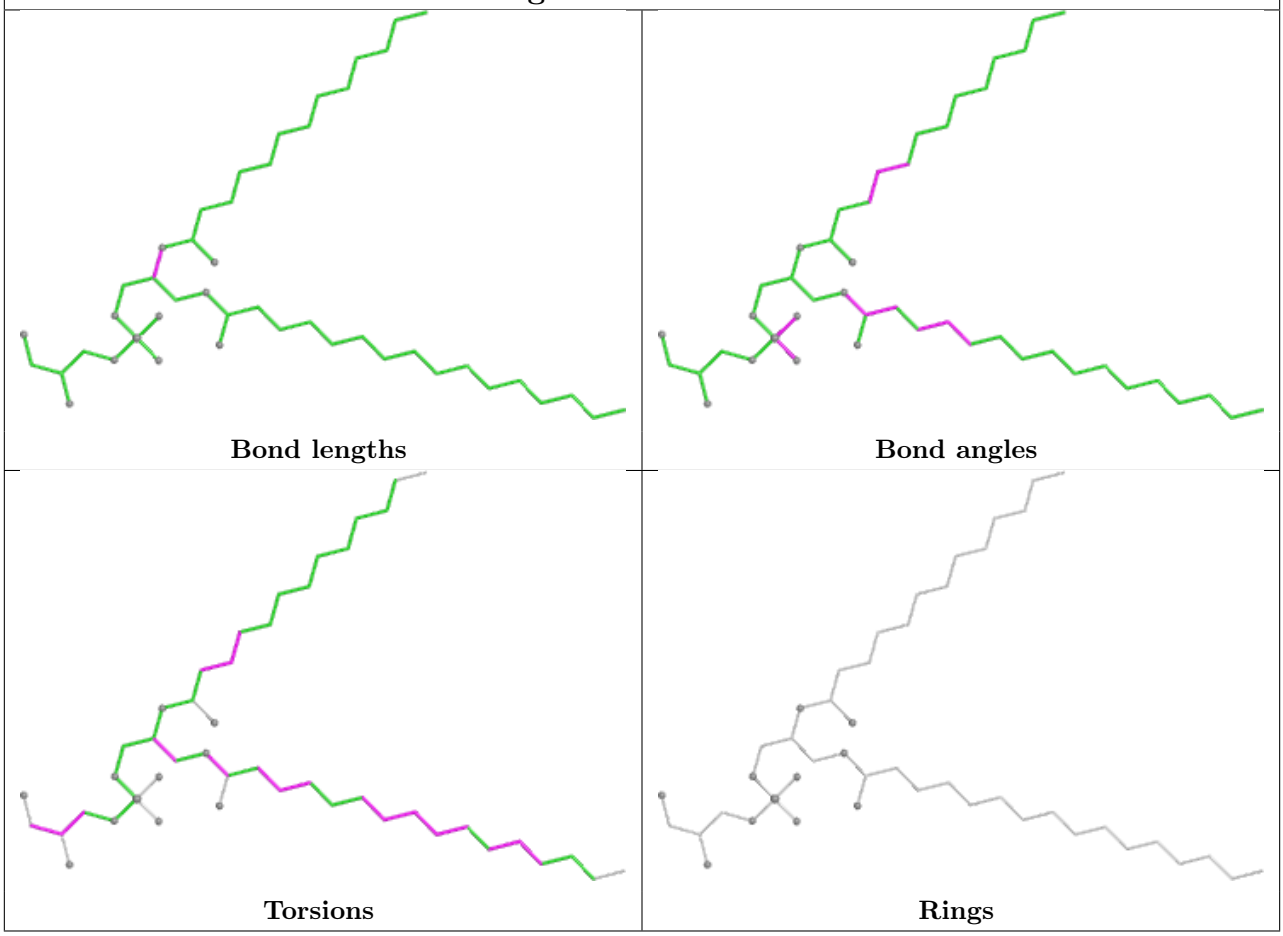
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 2 405



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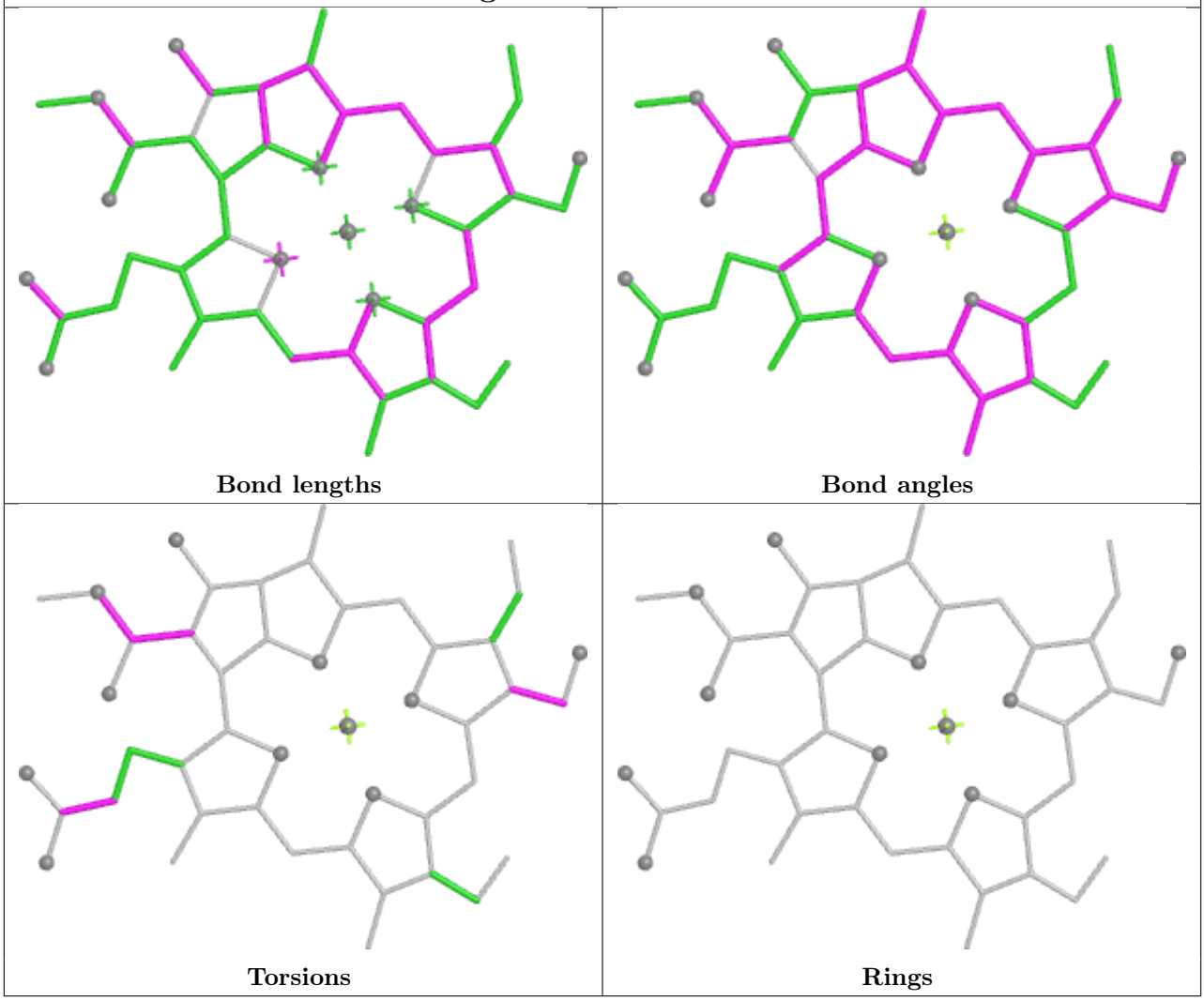
Ligand CHL BV 605



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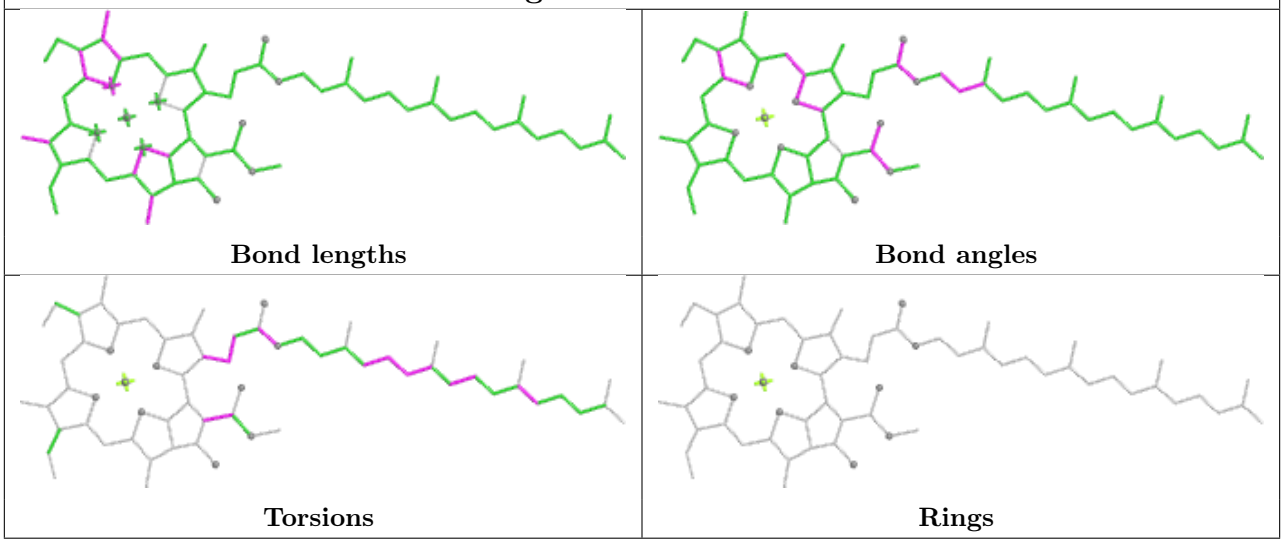

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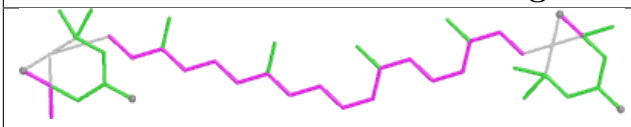
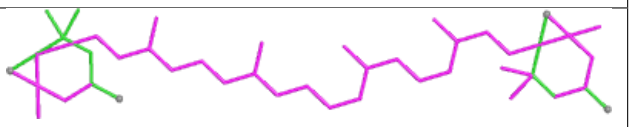
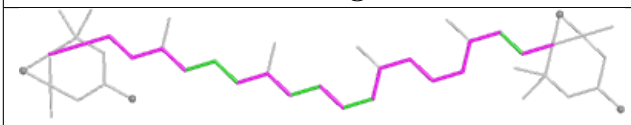
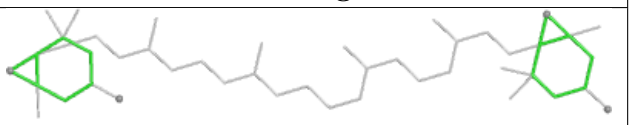
 Bond lengths	 Bond angles
 Torsions	 Rings

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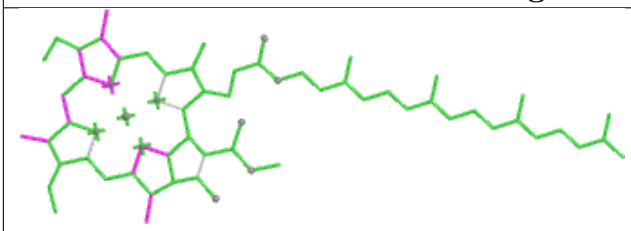
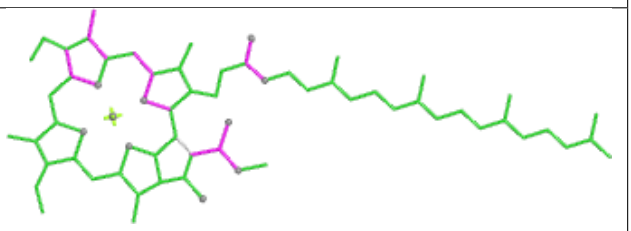
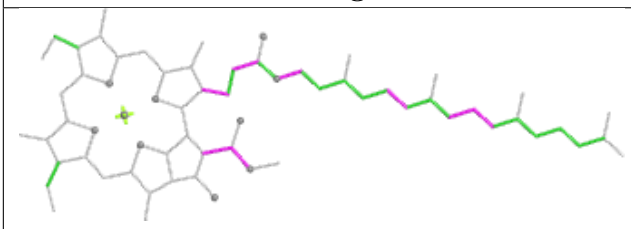
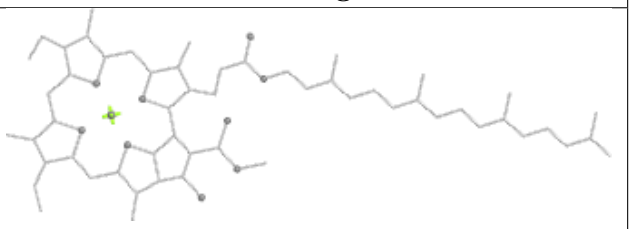
 Bond lengths	 Bond angles
 Torsions	 Rings

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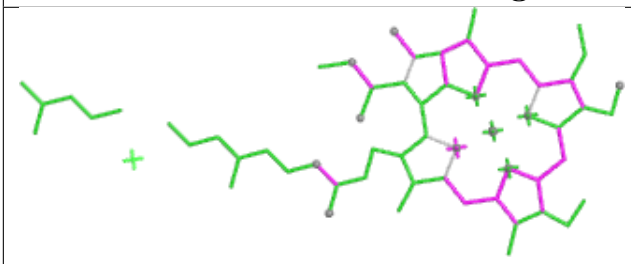
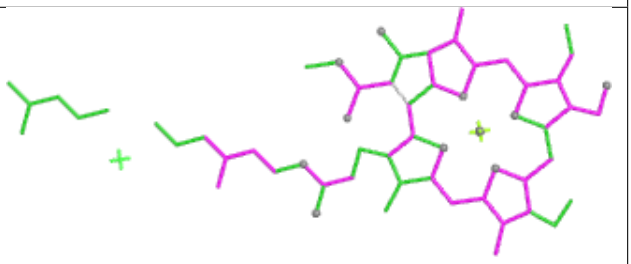
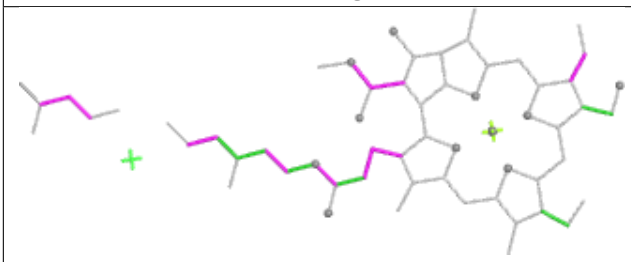
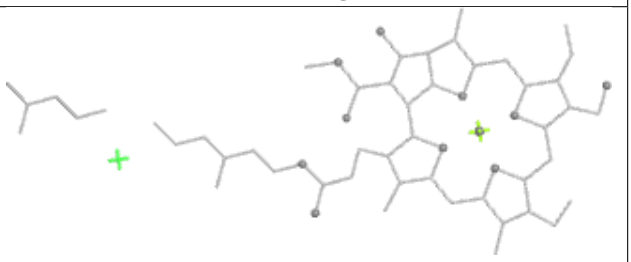
 Bond lengths	 Bond angles
 Torsions	 Rings

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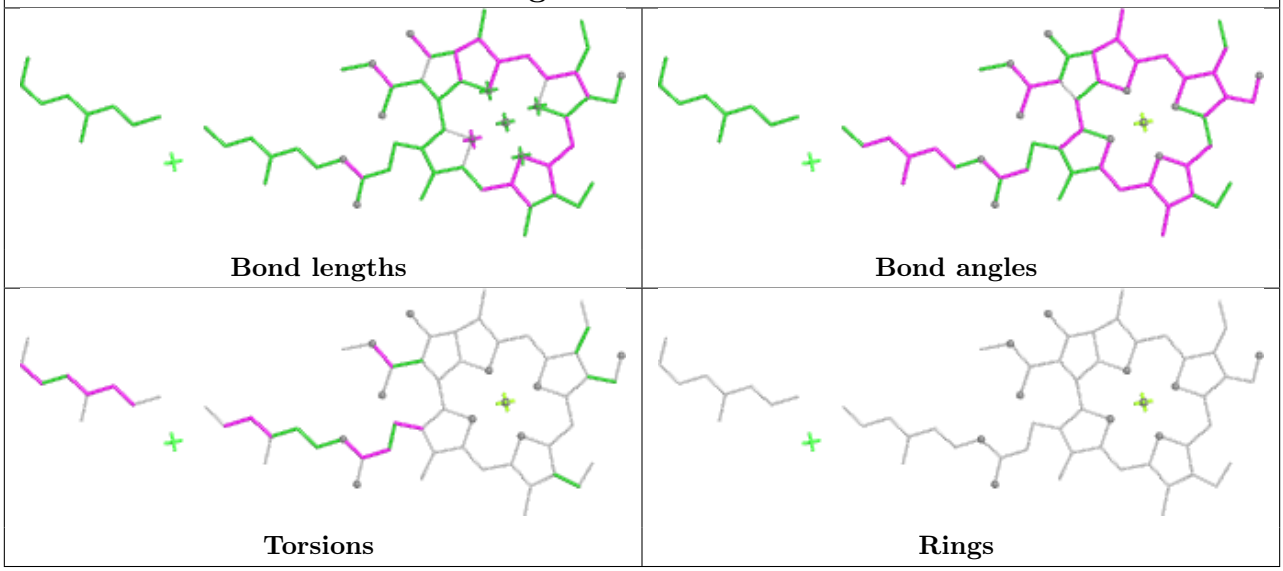
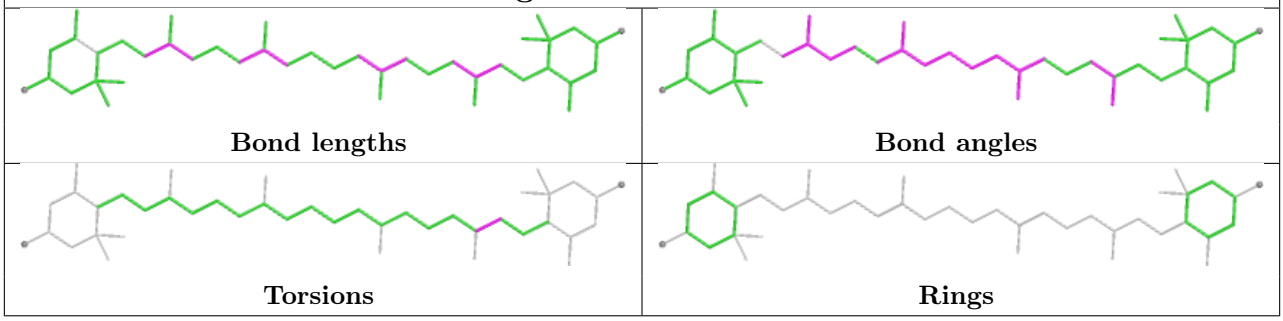
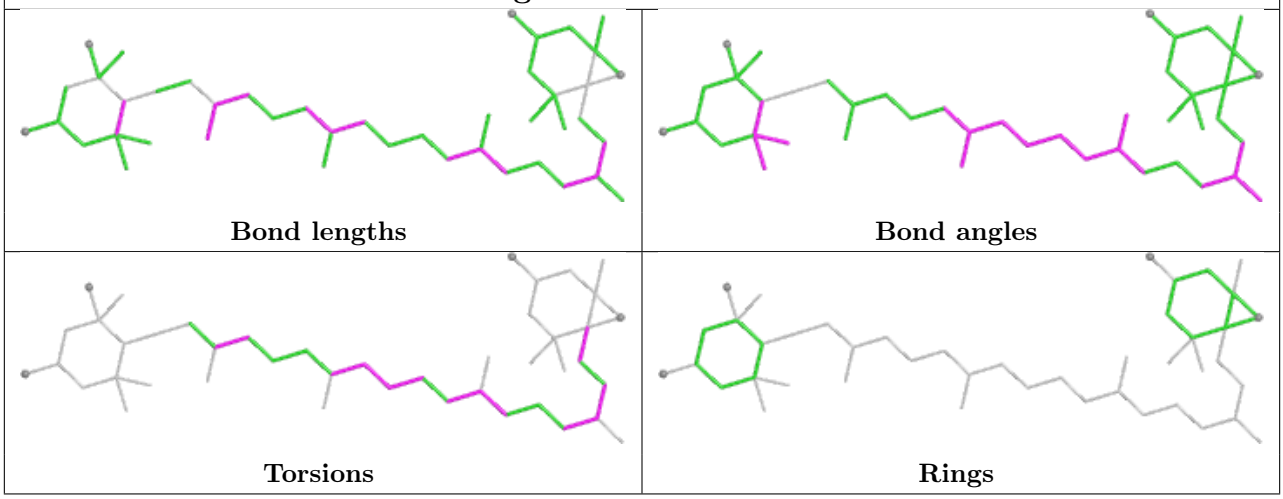


Ligand LUT A6 614



Ligand NEX A2 617



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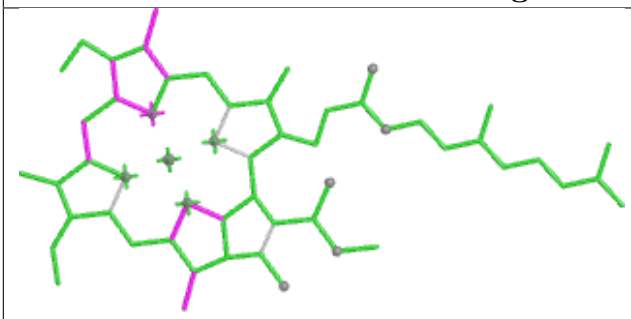
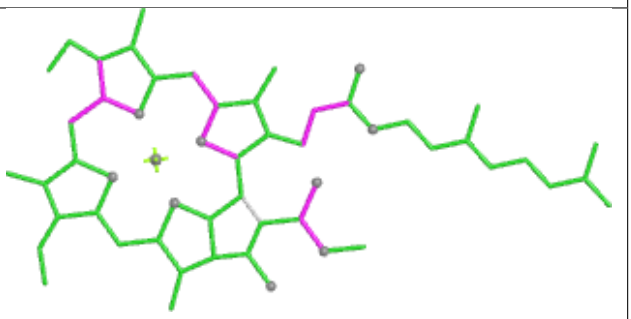
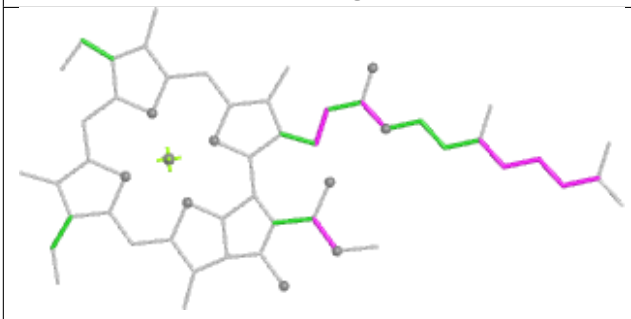
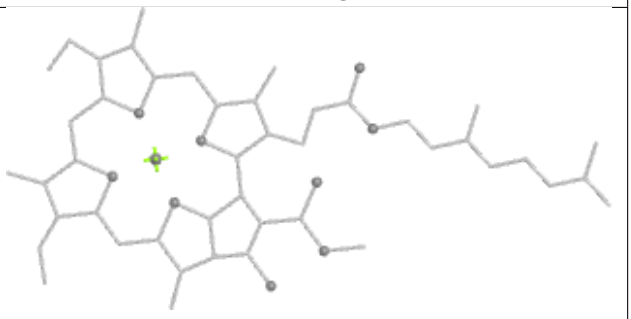
 Bond lengths	 Bond angles
 Torsions	 Rings

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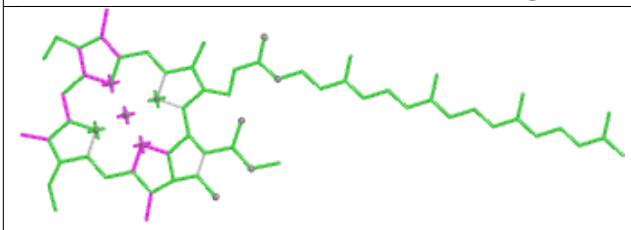
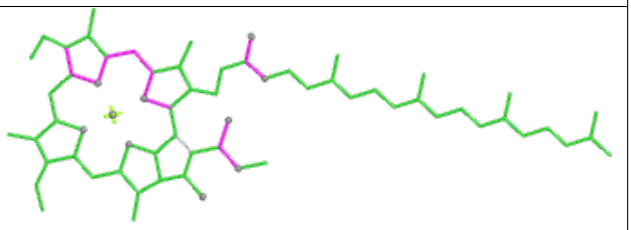
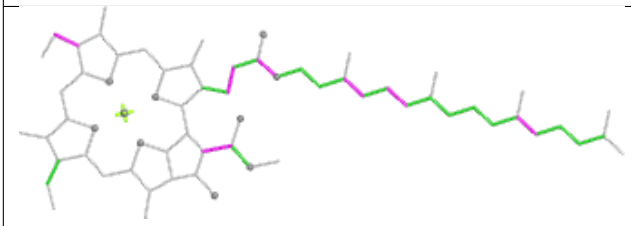
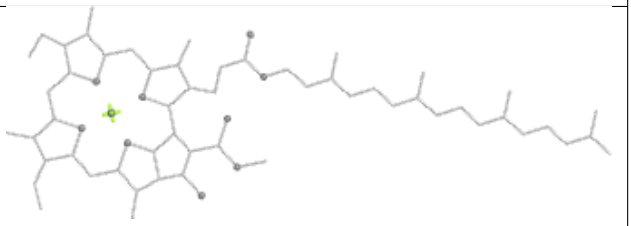
 Bond lengths	 Bond angles
 Torsions	 Rings

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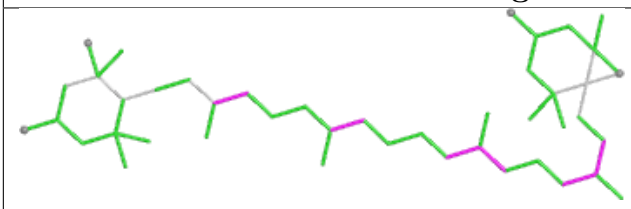
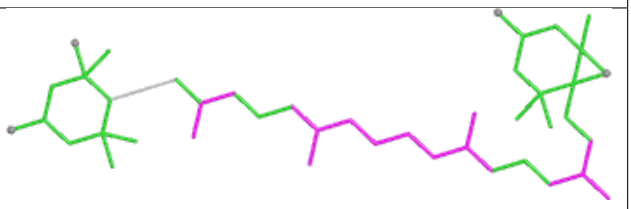
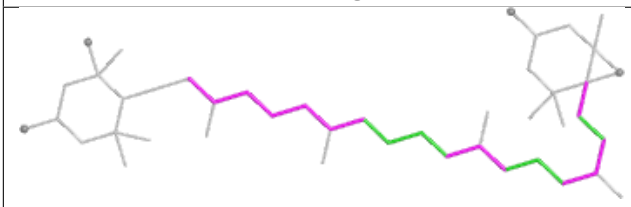


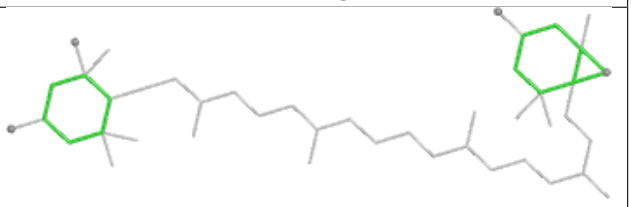
Bond lengths



Bond angles

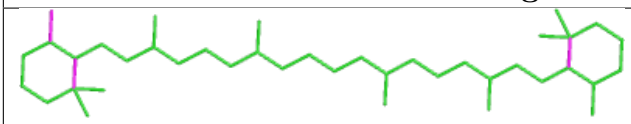


Torsions



Rings

Ligand BCR K 102



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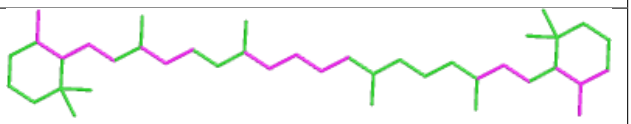
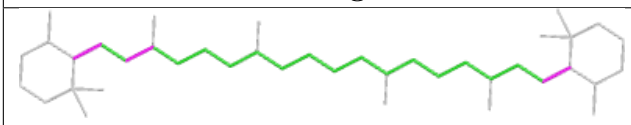


Bond angles



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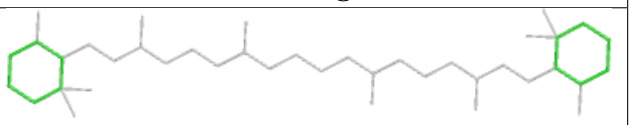
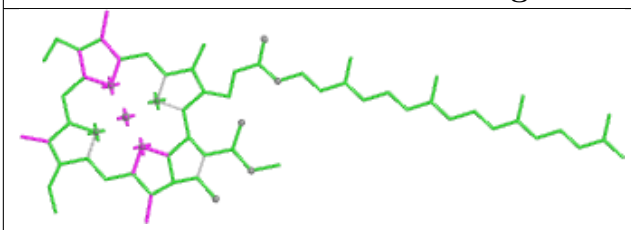


Rings

Ligand CLA BU 609



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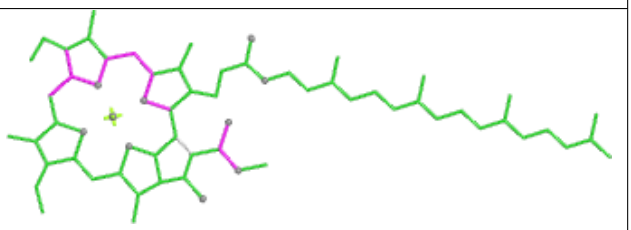

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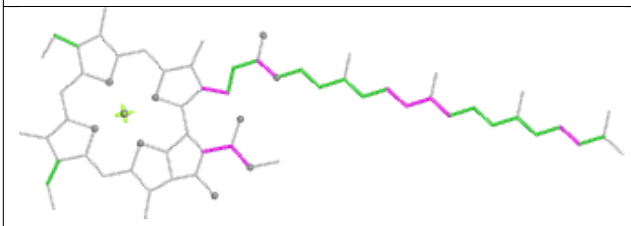

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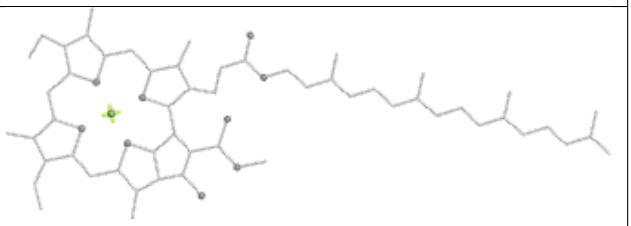
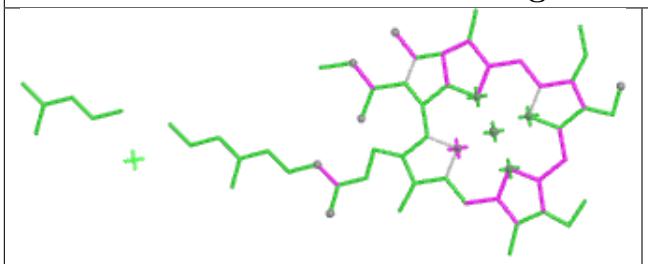


Rings

Ligand CHL 7 310



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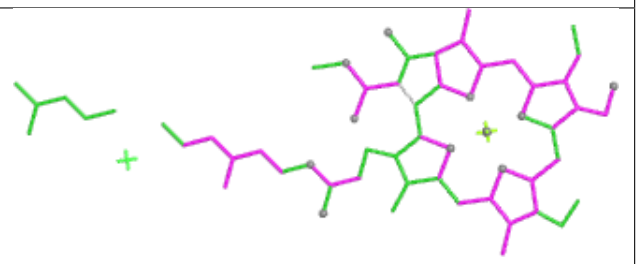

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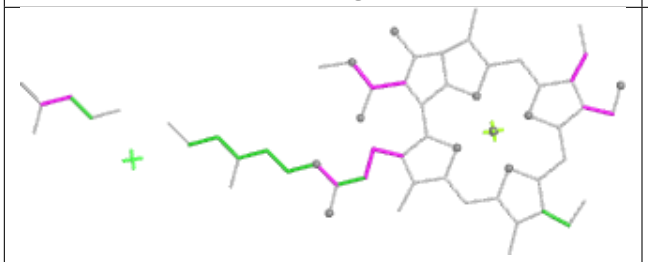

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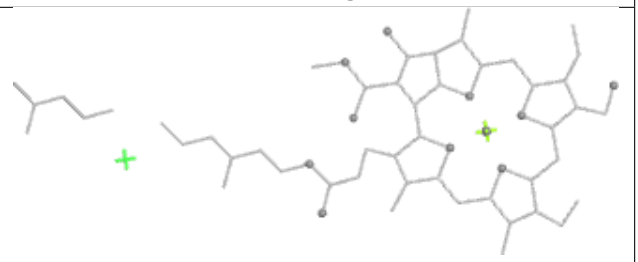
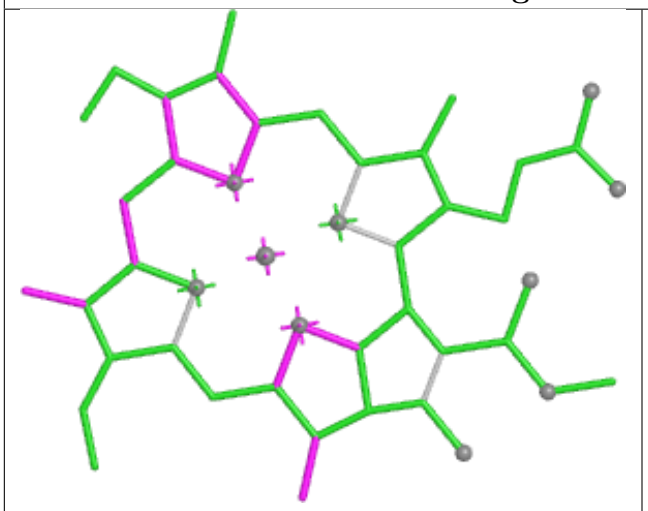


Rings

Ligand CLA AB 308



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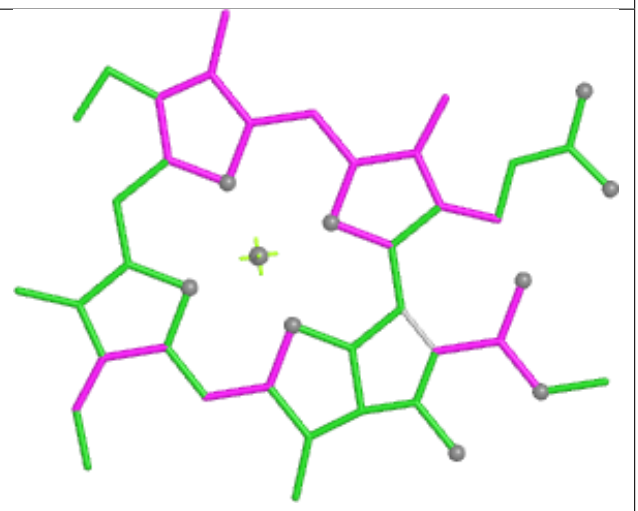
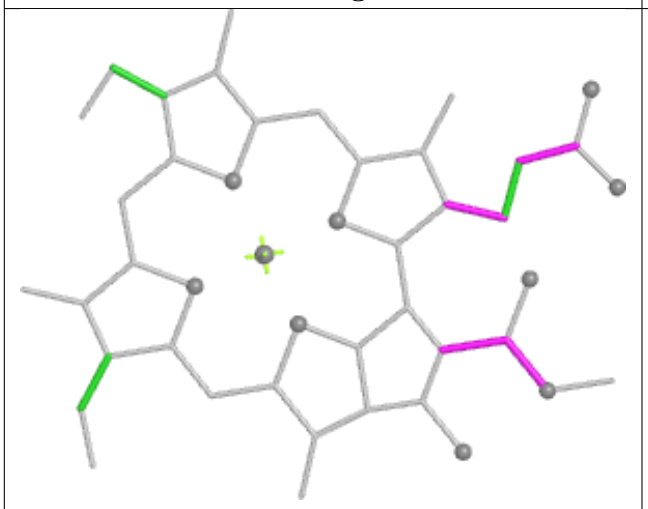


Bond angles



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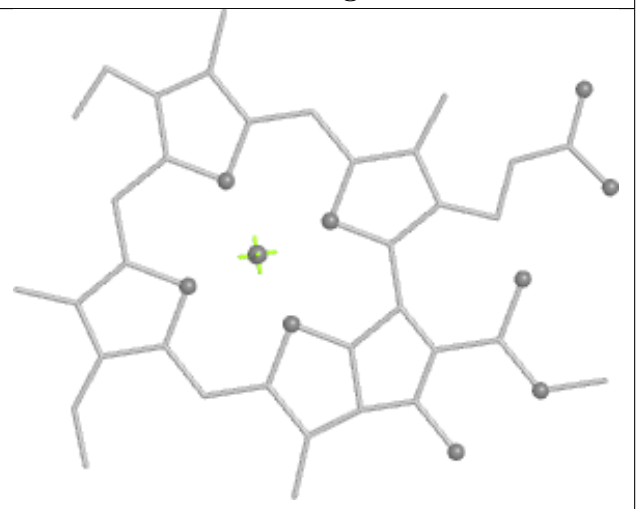
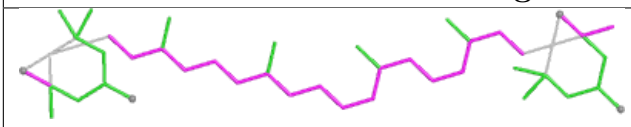
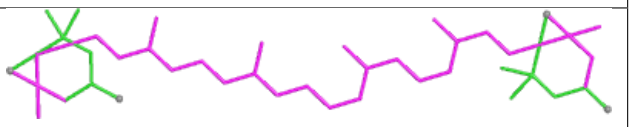
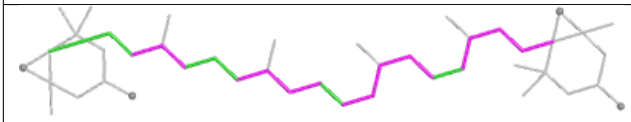
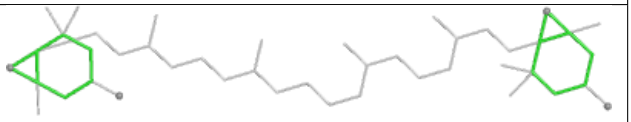


Rings

Ligand XAT A2 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

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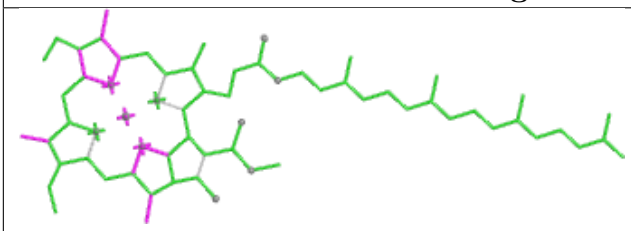
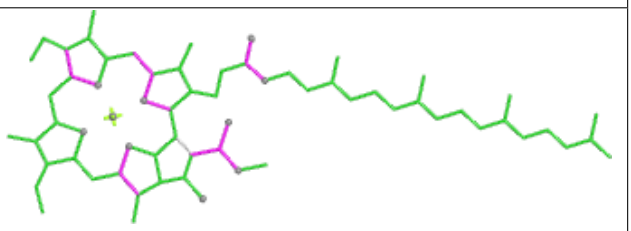
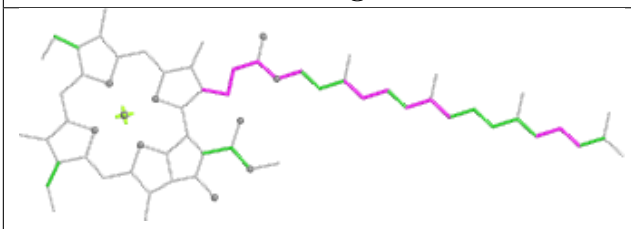
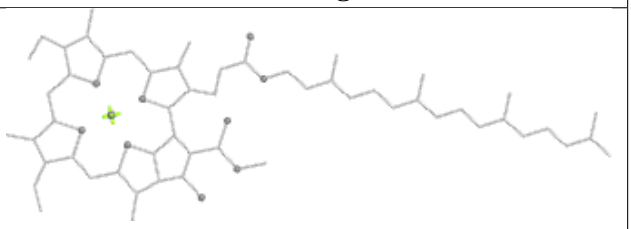
 Bond lengths	 Bond angles
 Torsions	 Rings

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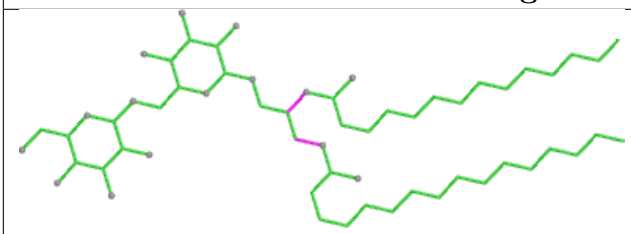
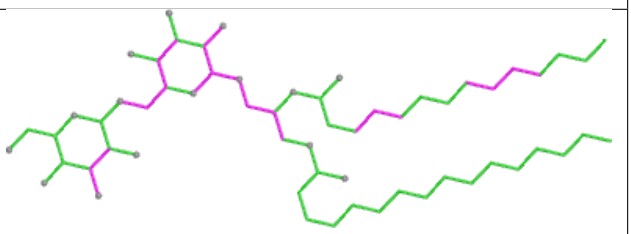
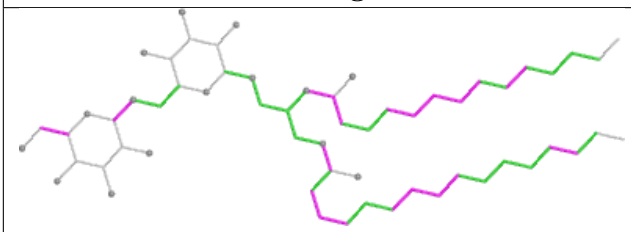
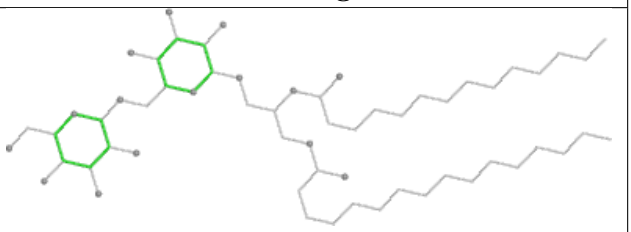
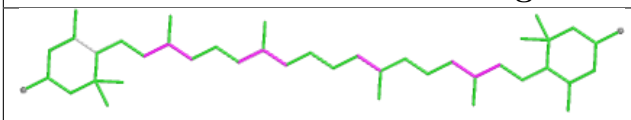
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT BJ 616



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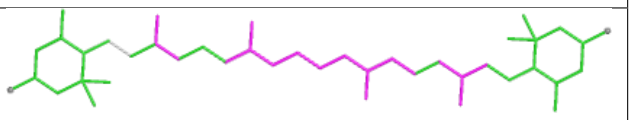

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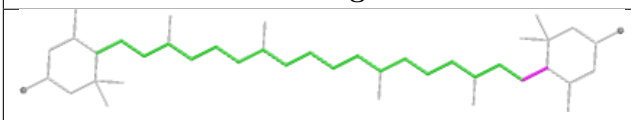

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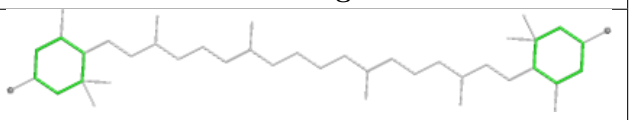
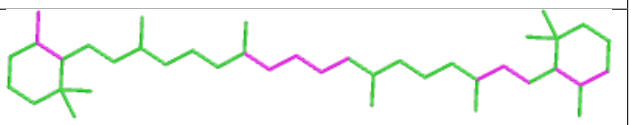


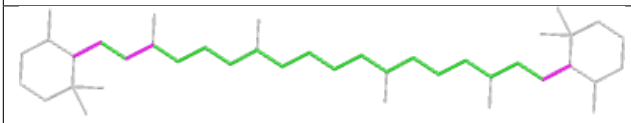
Rings

Ligand BCR a 411

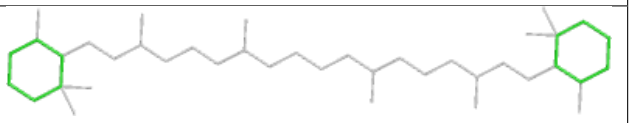
Bond lengths



Bond angles

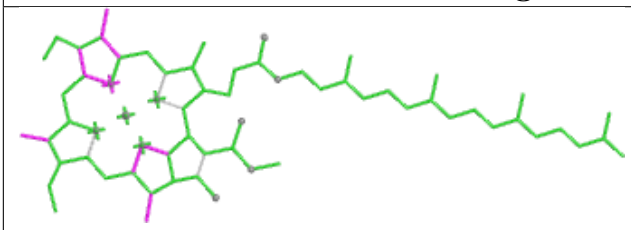


Torsions



Rings

Ligand CLA A2 603



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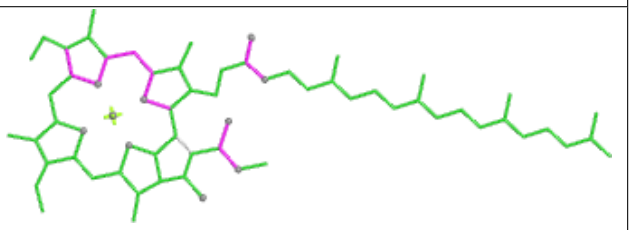

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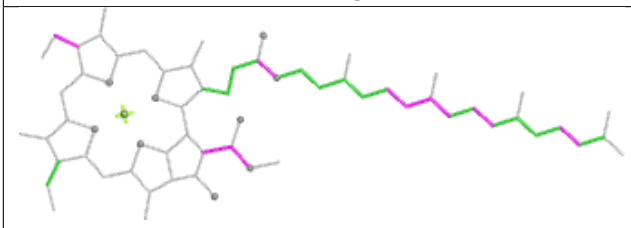

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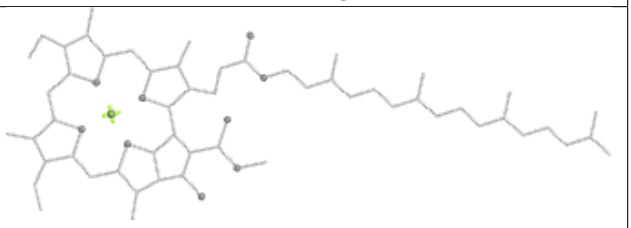
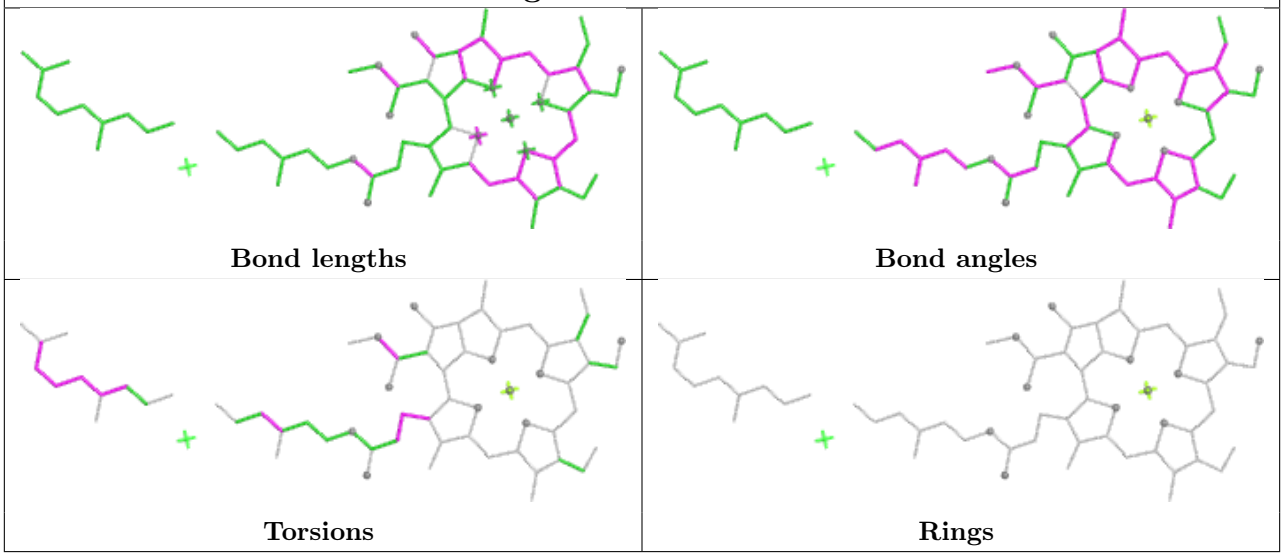
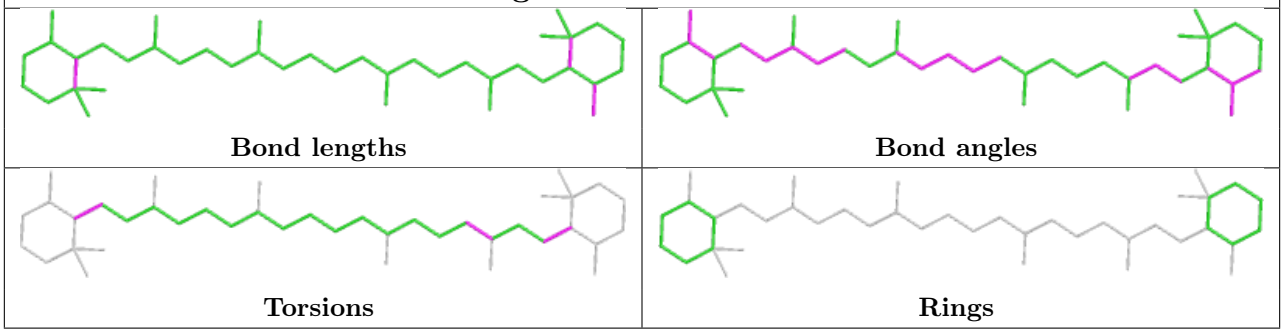


Rings

Ligand CHL G 607



Ligand BCR BF 516



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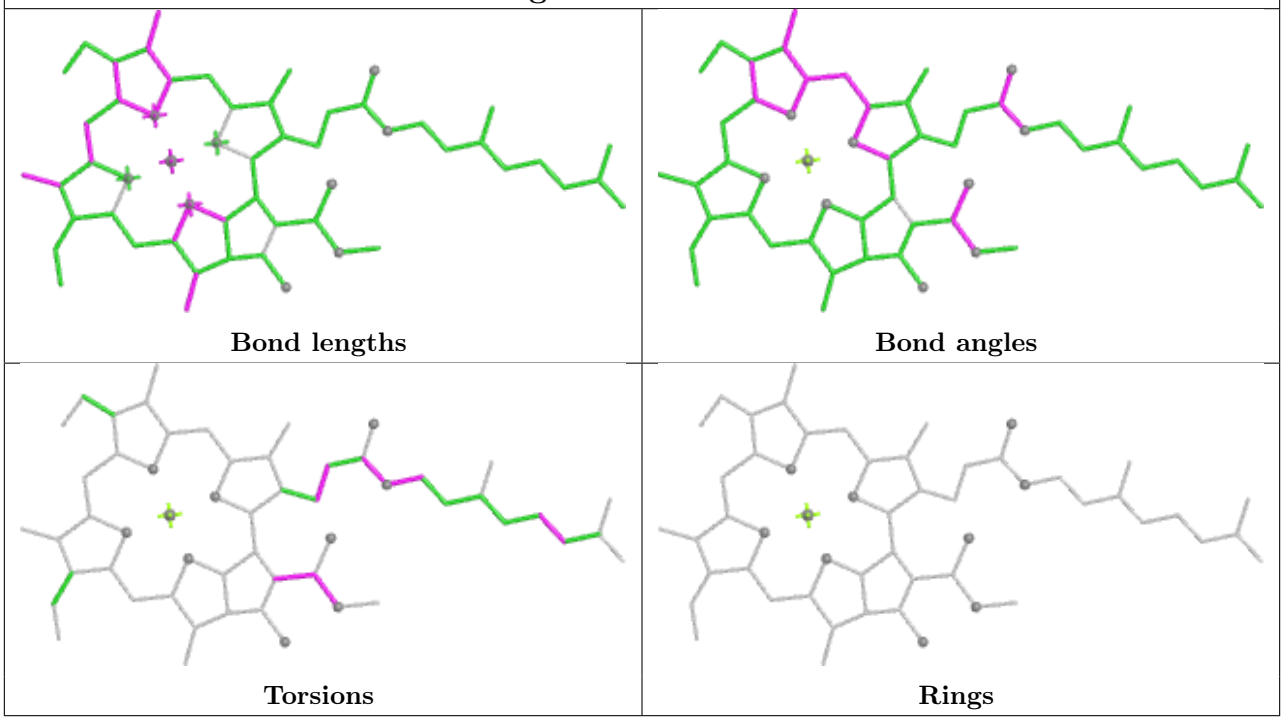
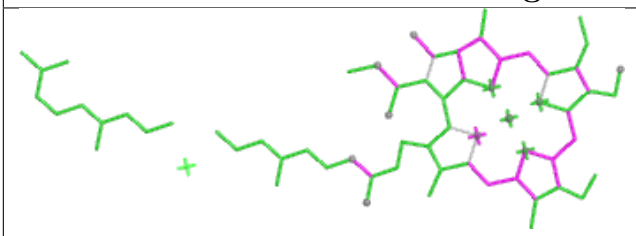
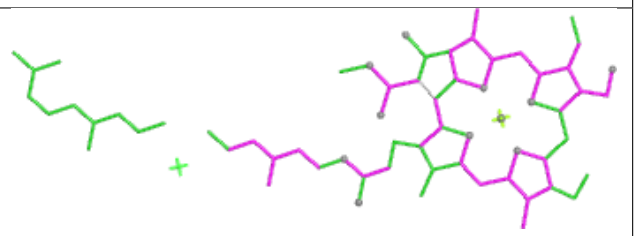
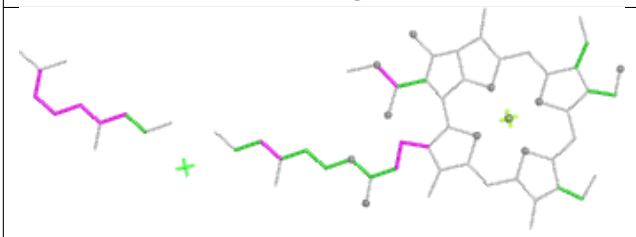
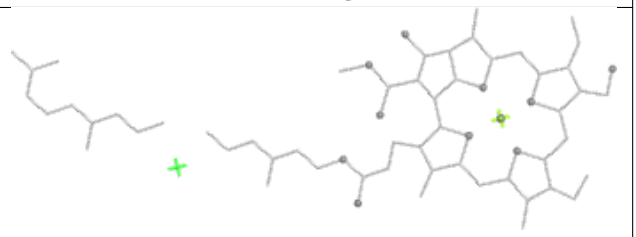


Ligand CHL Y 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

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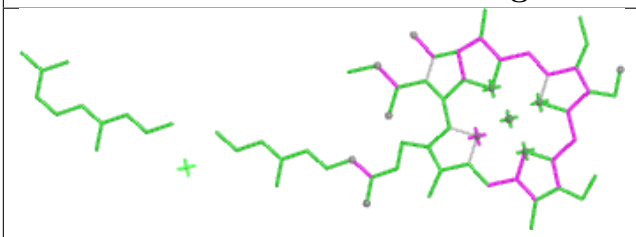
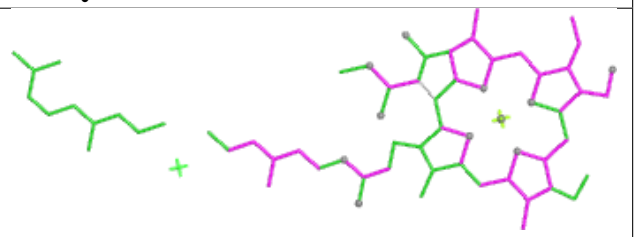
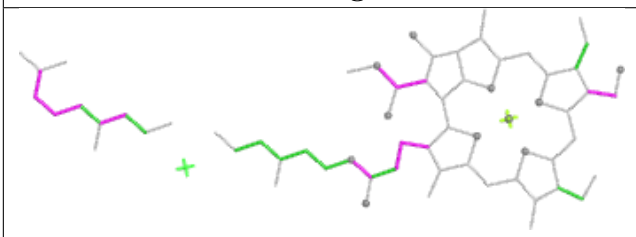
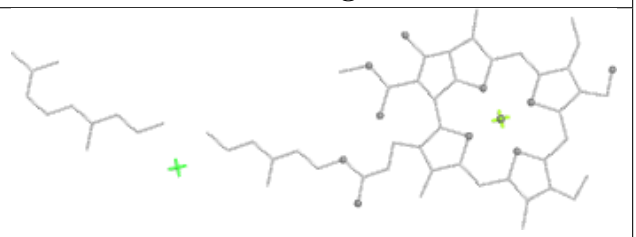
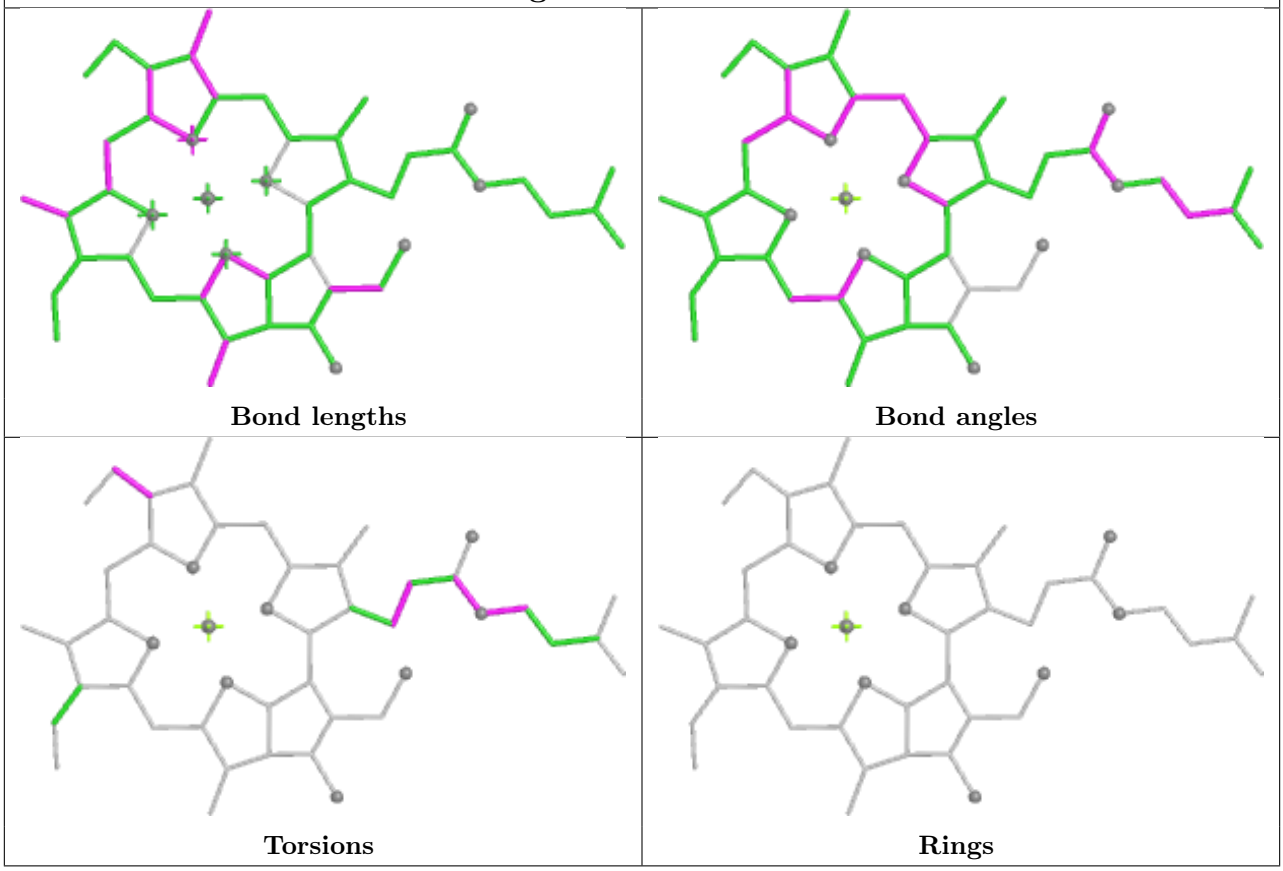
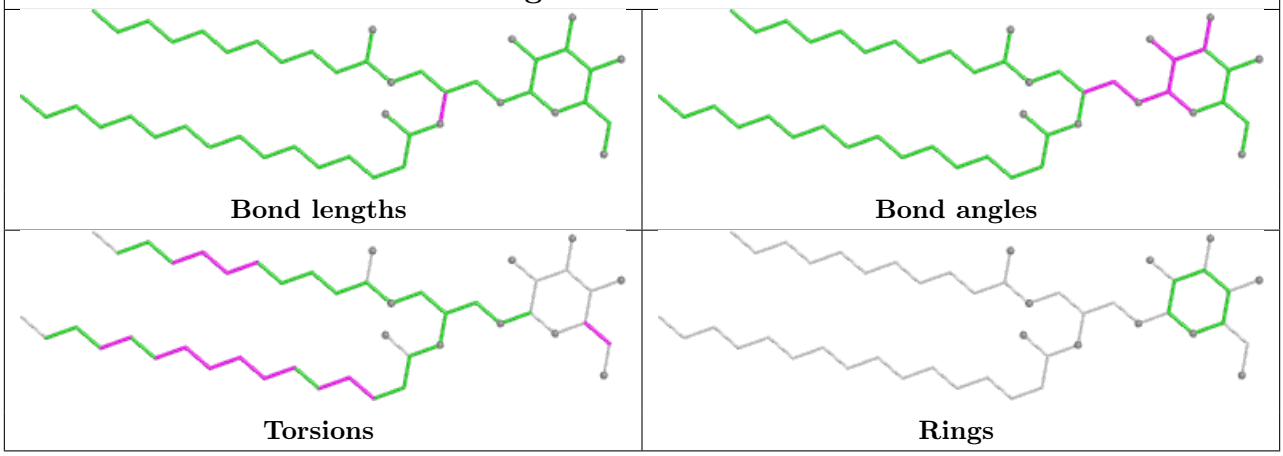
 Bond lengths	 Bond angles
 Torsions	 Rings

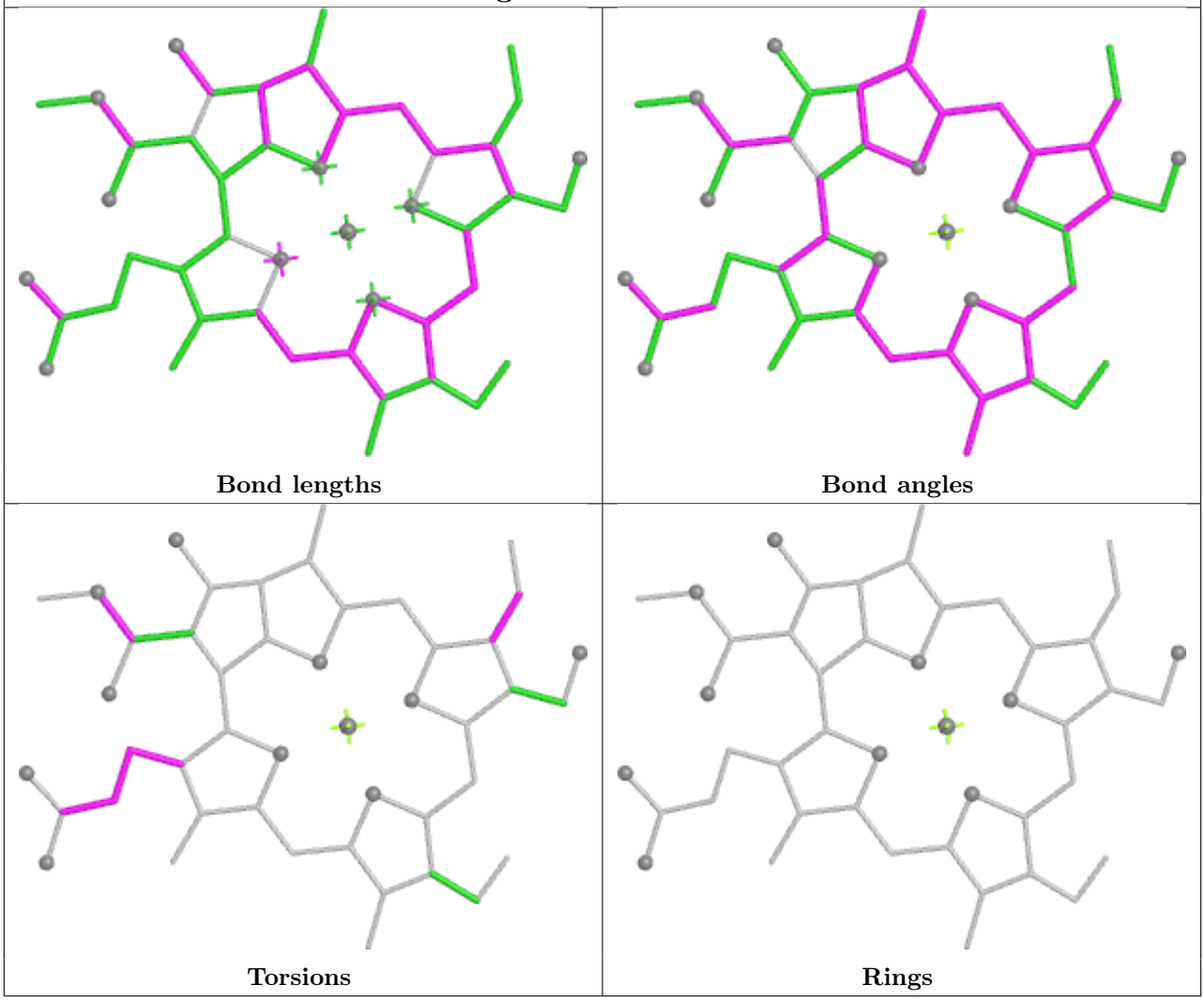
Ligand CLA 7 311



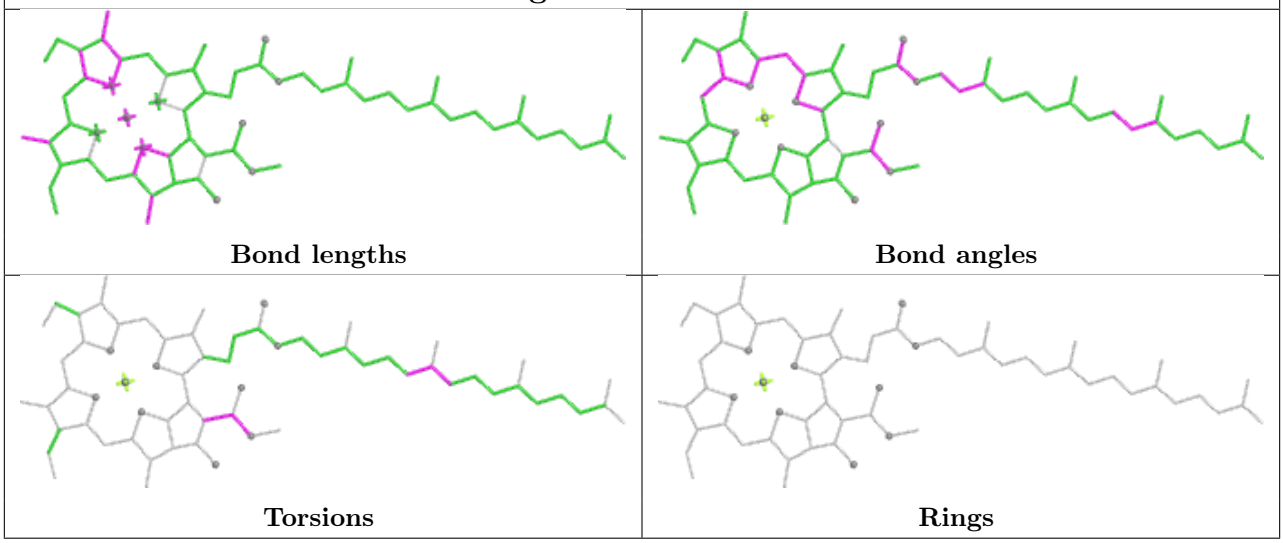
Ligand LMG 2 407



Ligand CHL 5 601



Ligand CLA 1 509



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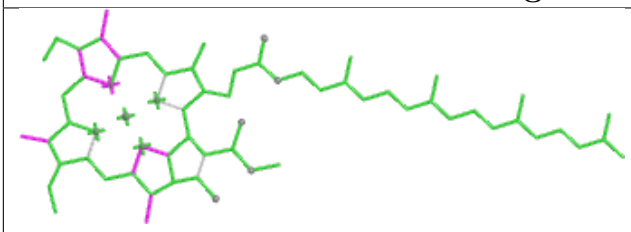
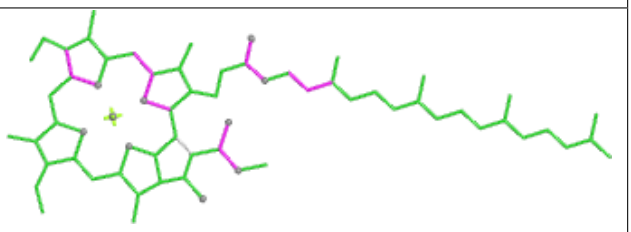
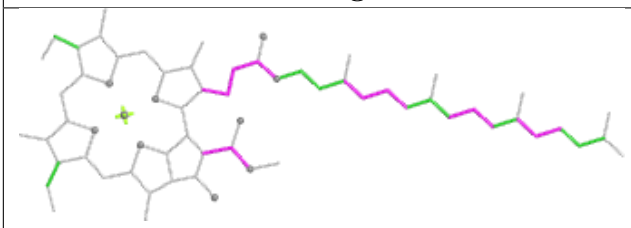
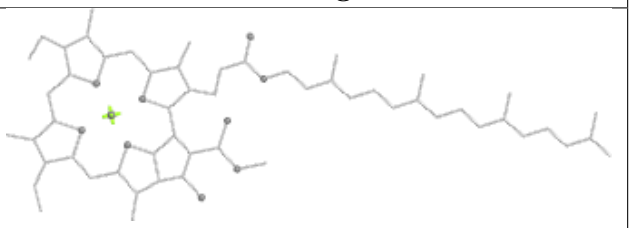
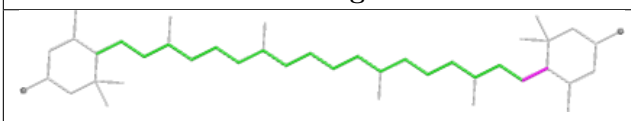
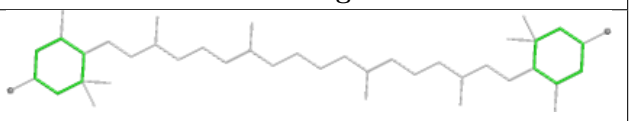
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 9 616	
Bond lengths	Bond angles
 Torsions	 Rings

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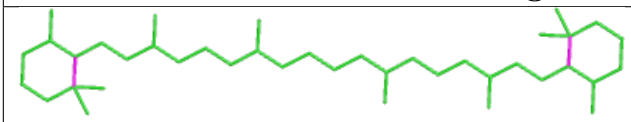
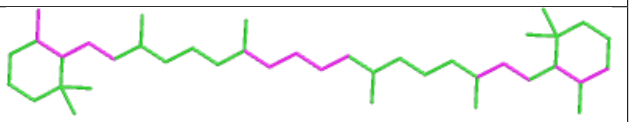
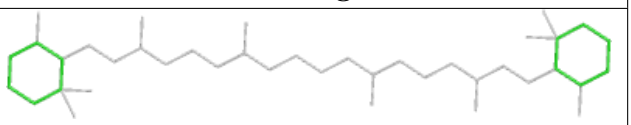
 Bond lengths	 Bond angles
Torsions	 Rings

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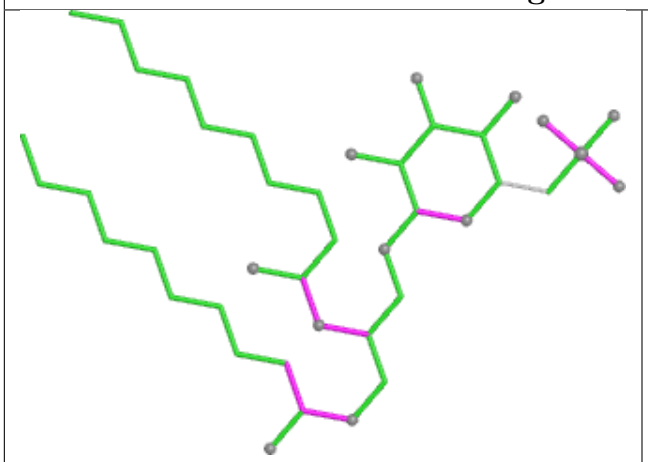

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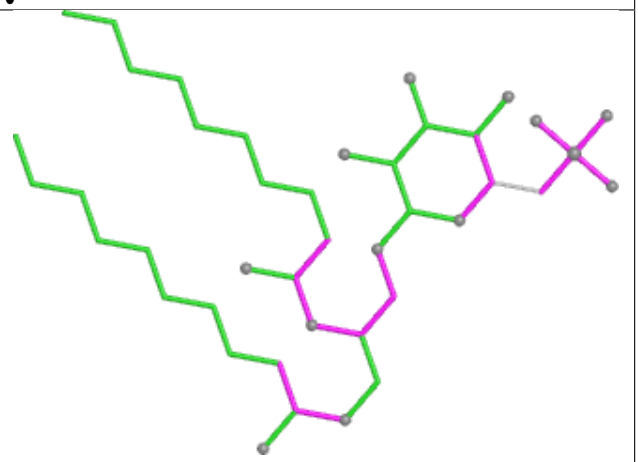

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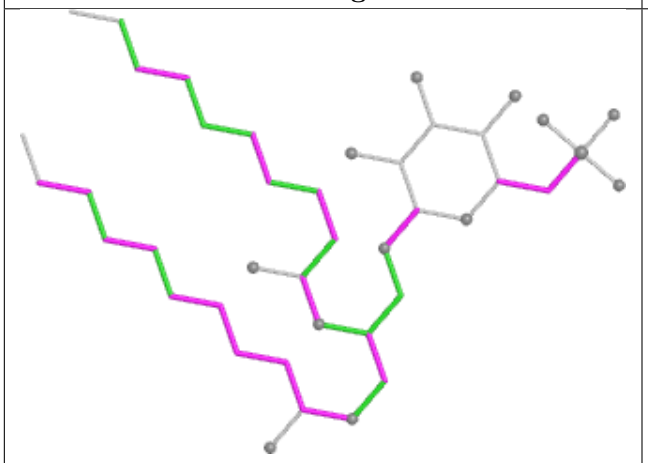

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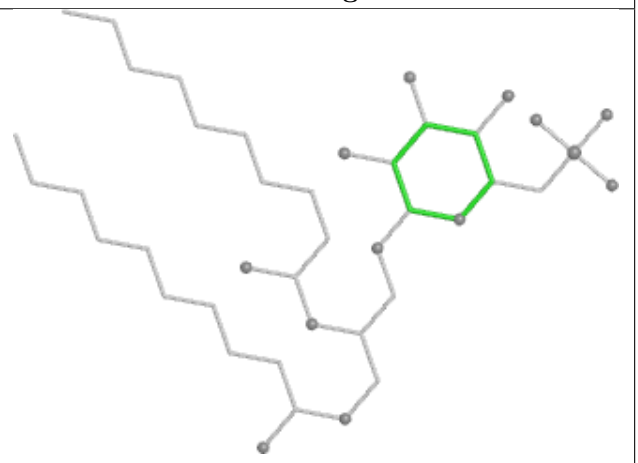

Rings

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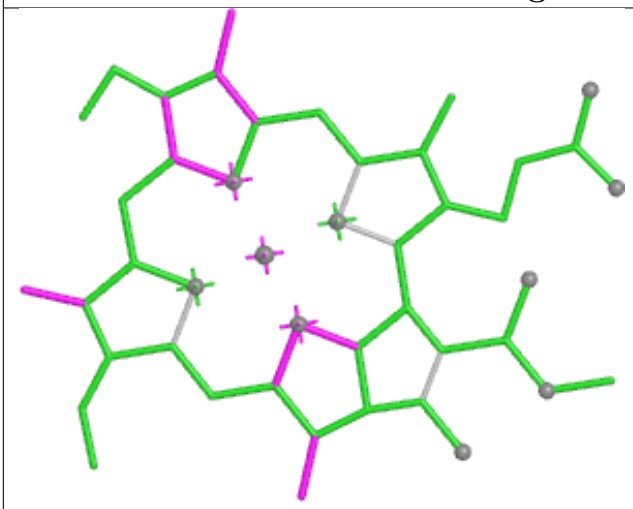

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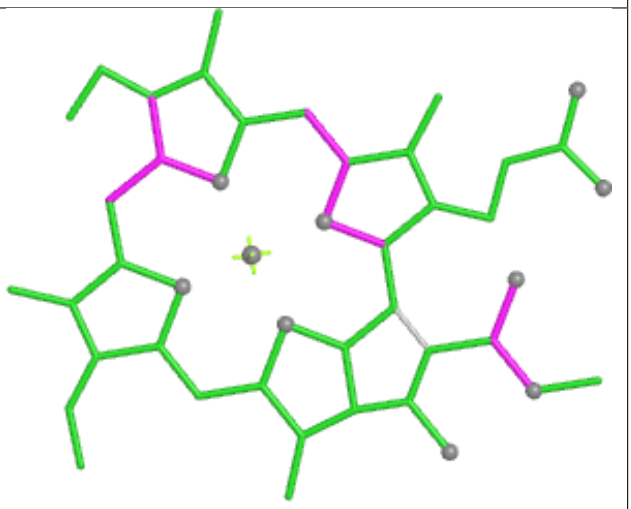

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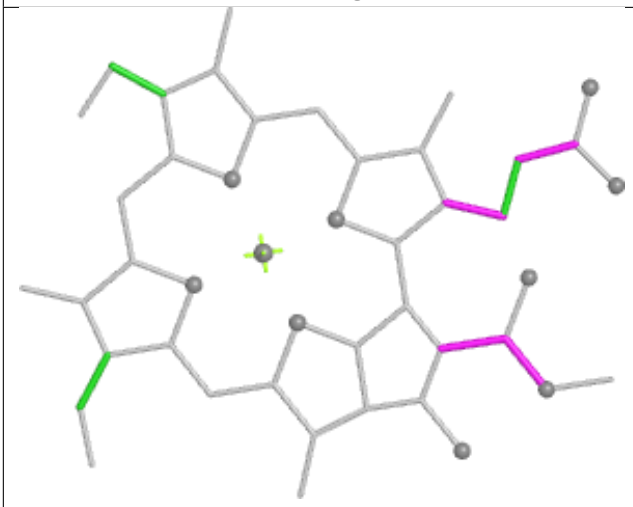
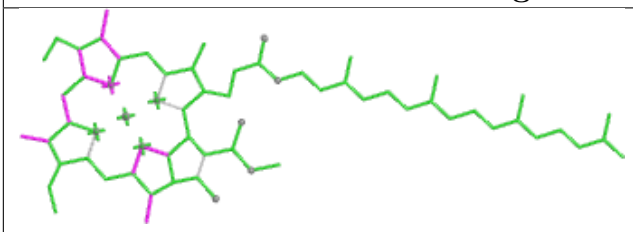


Torsions

Rings

Ligand CLA BE 616



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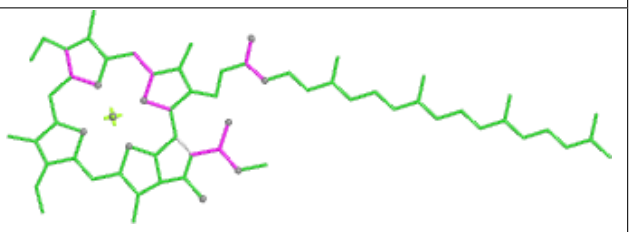

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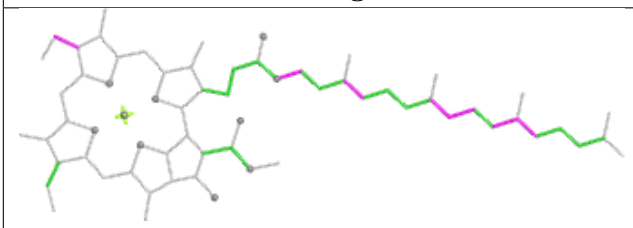

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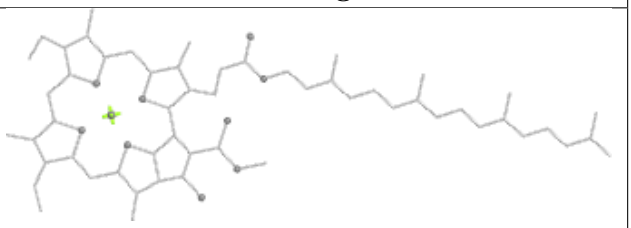

Rings

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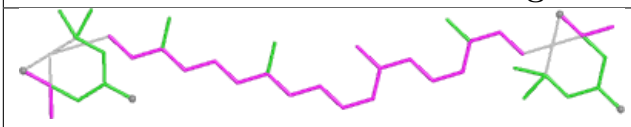
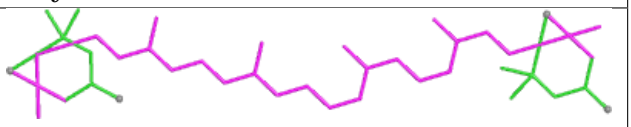
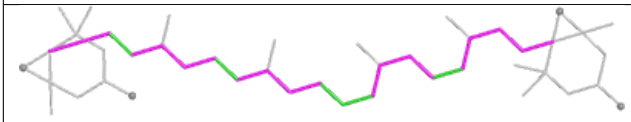
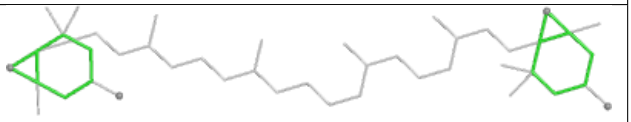
 Bond lengths	 Bond angles
 Torsions	 Rings

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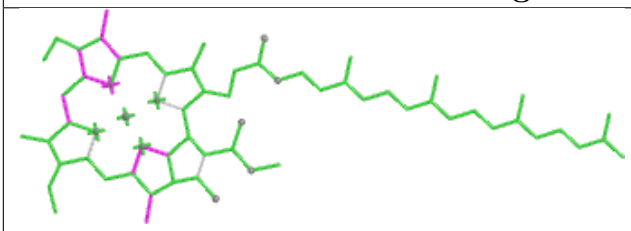
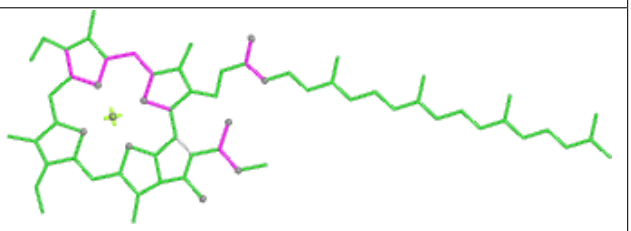
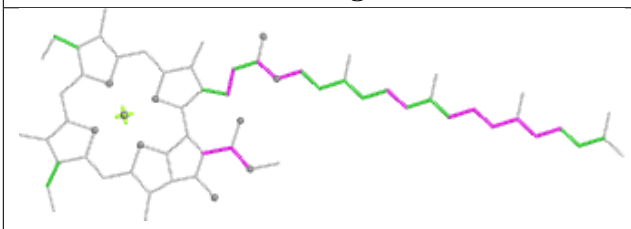
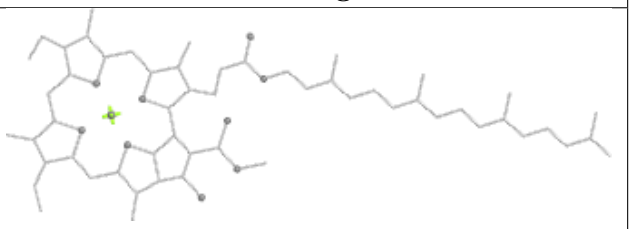
 Bond lengths	 Bond angles
 Torsions	 Rings

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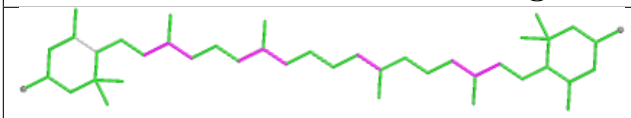
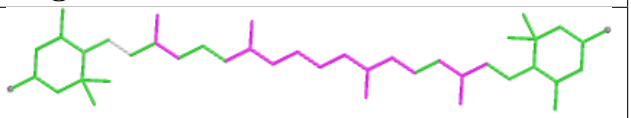
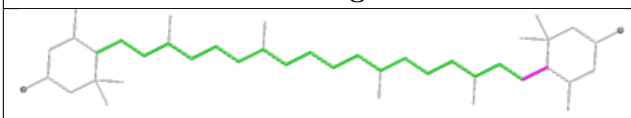
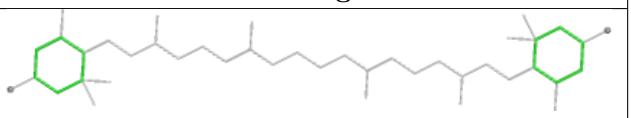
 Bond lengths	 Bond angles
 Torsions	 Rings

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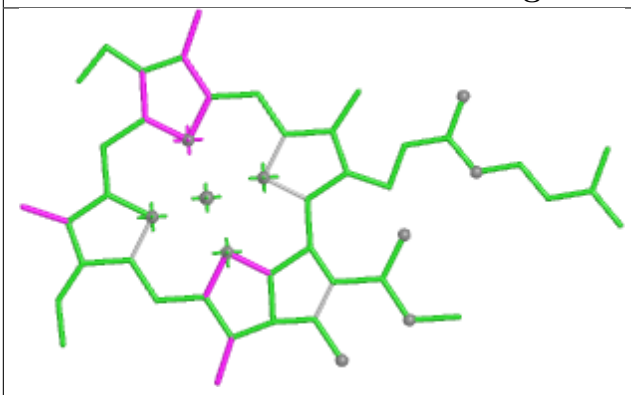
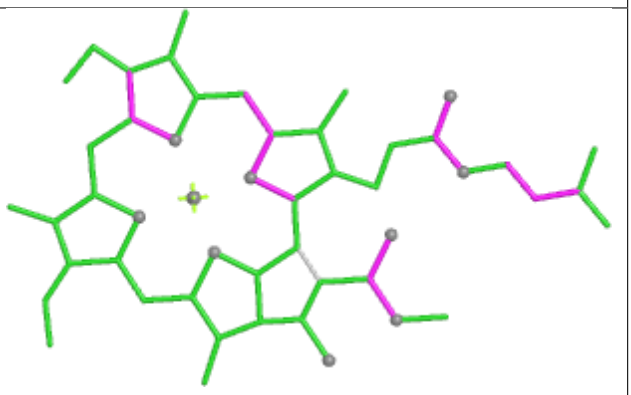
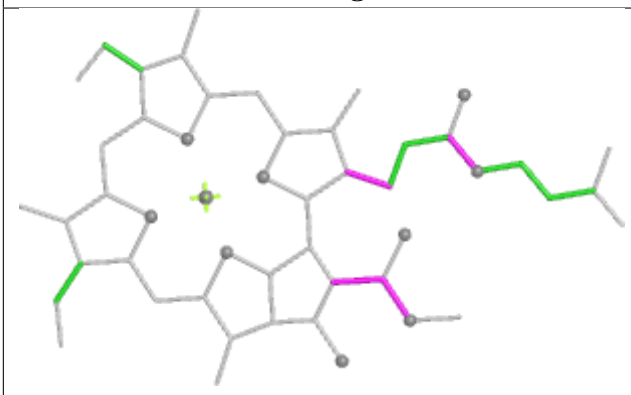
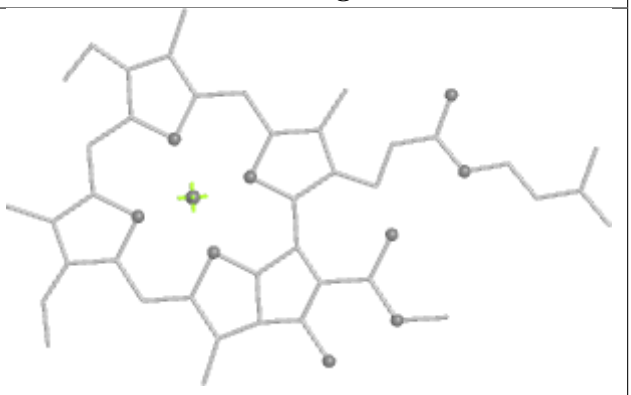
 Bond lengths	 Bond angles
 Torsions	 Rings

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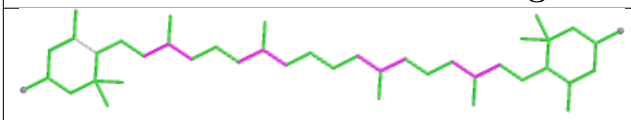
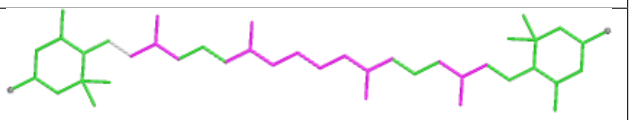
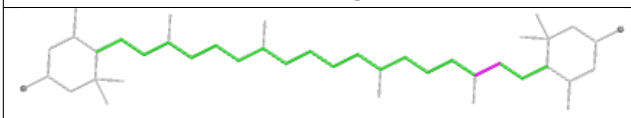
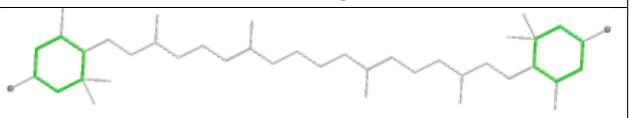
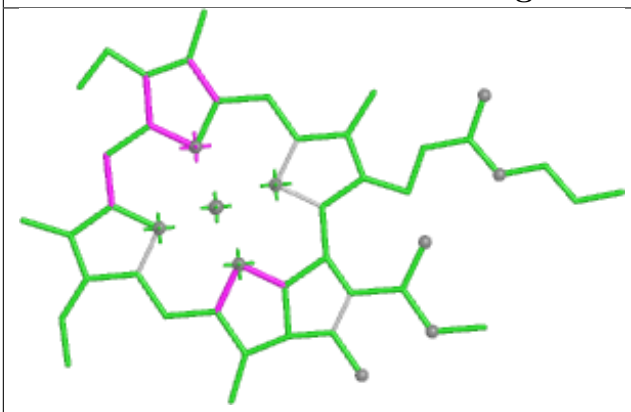
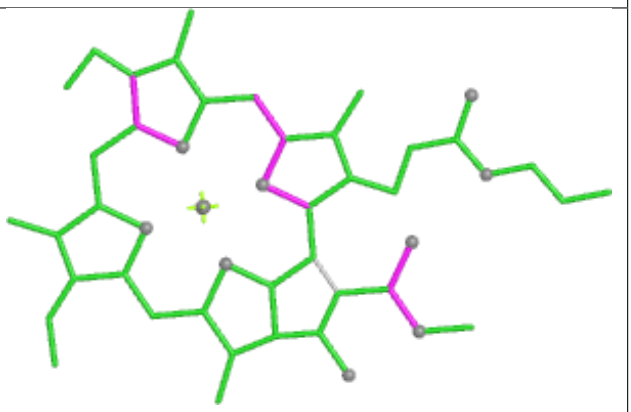
 Bond lengths	 Bond angles
 Torsions	 Rings

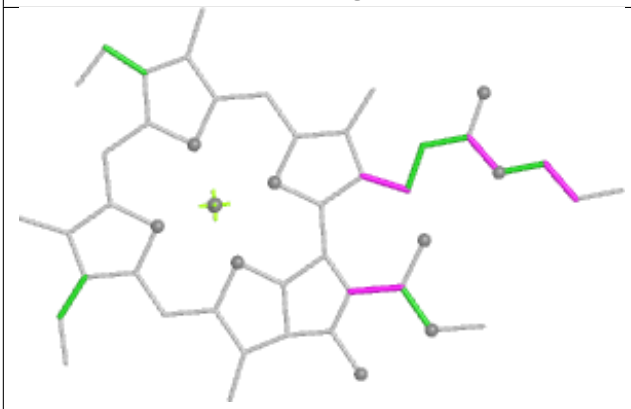
Ligand CLA BJ 614



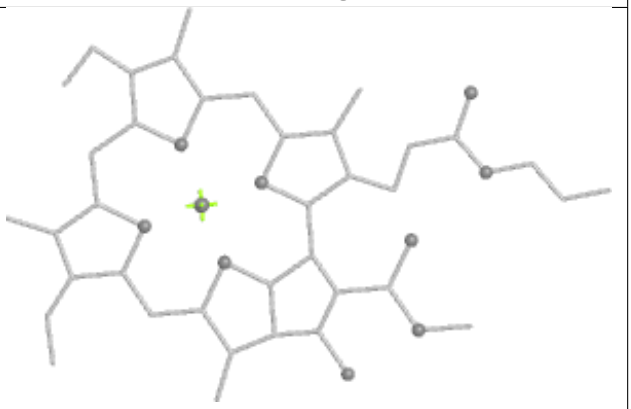
Bond lengths



Bond angles

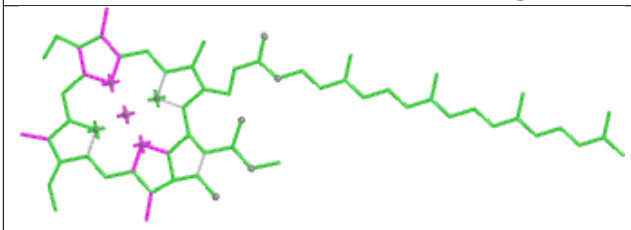


Torsions

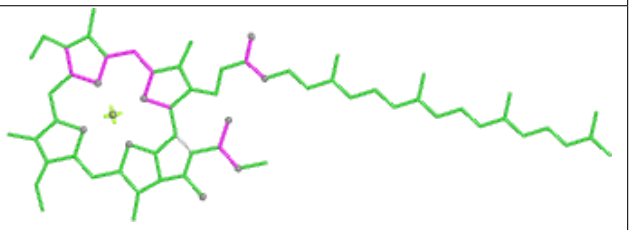


Rings

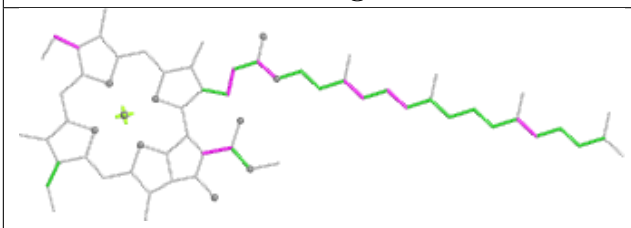
Ligand CLA BB 304



Bond lengths



Bond angles



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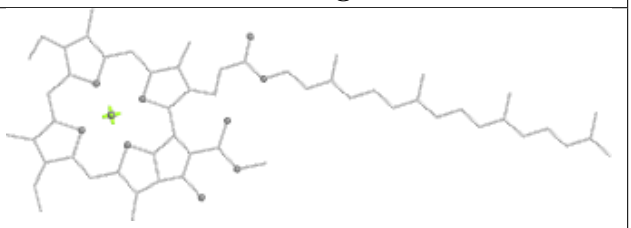
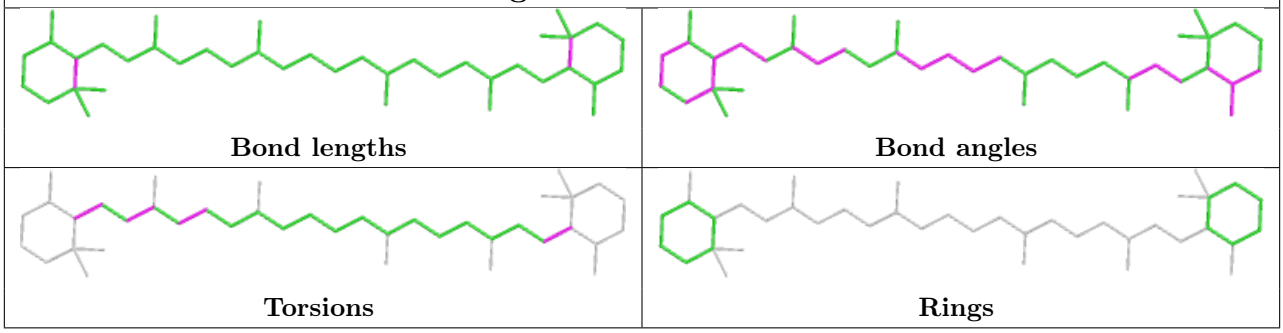
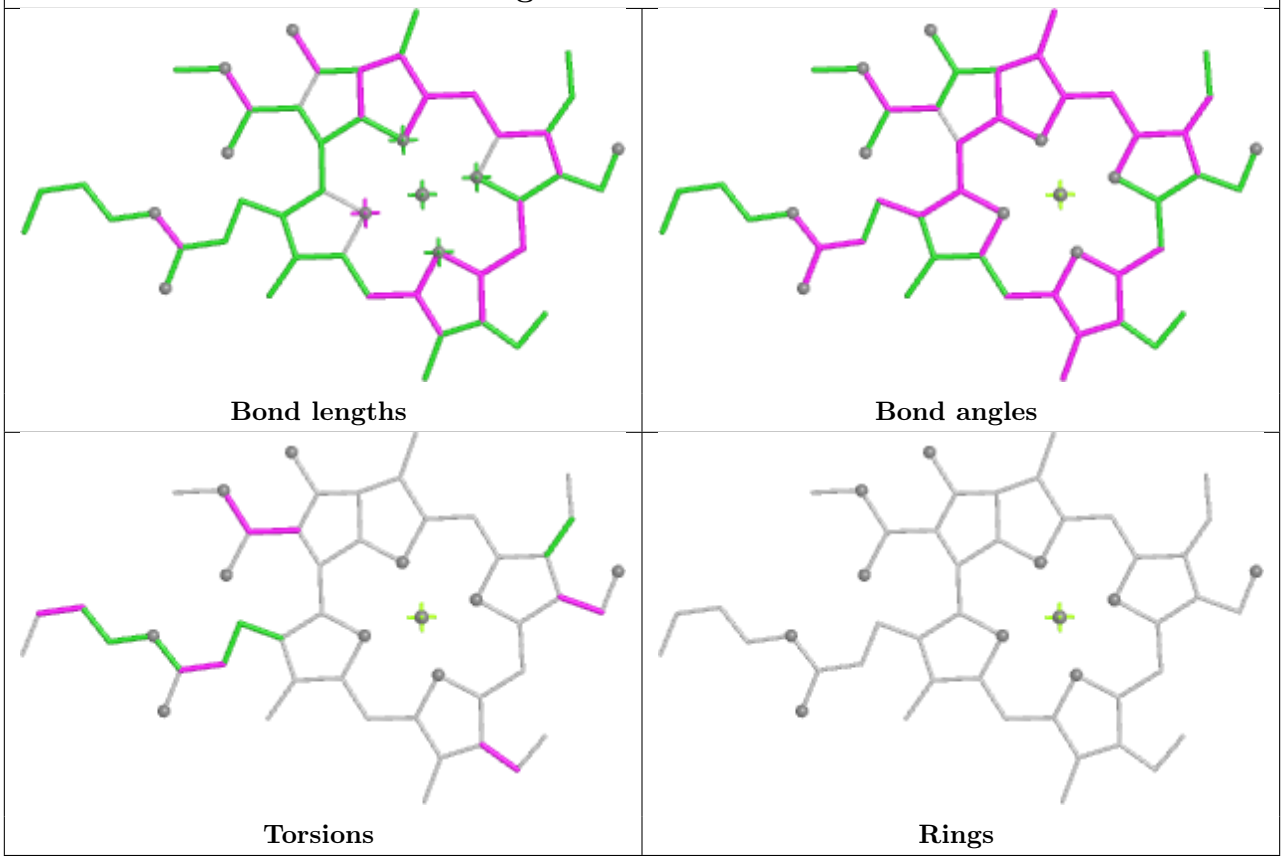


Rings

Ligand BCR BK 101



Ligand CHL Ba 307



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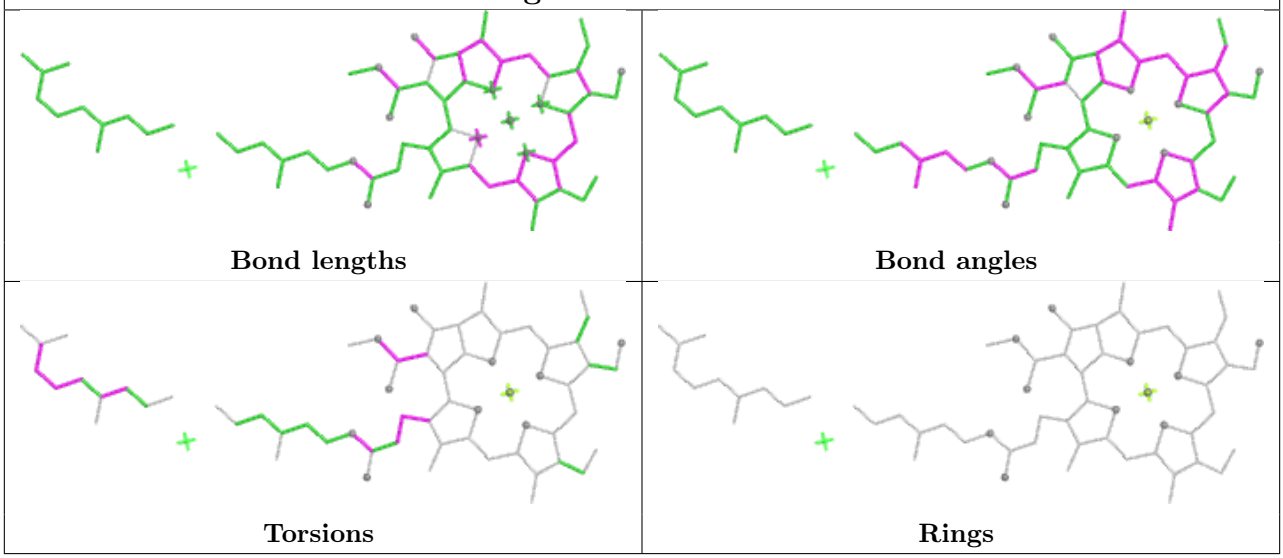
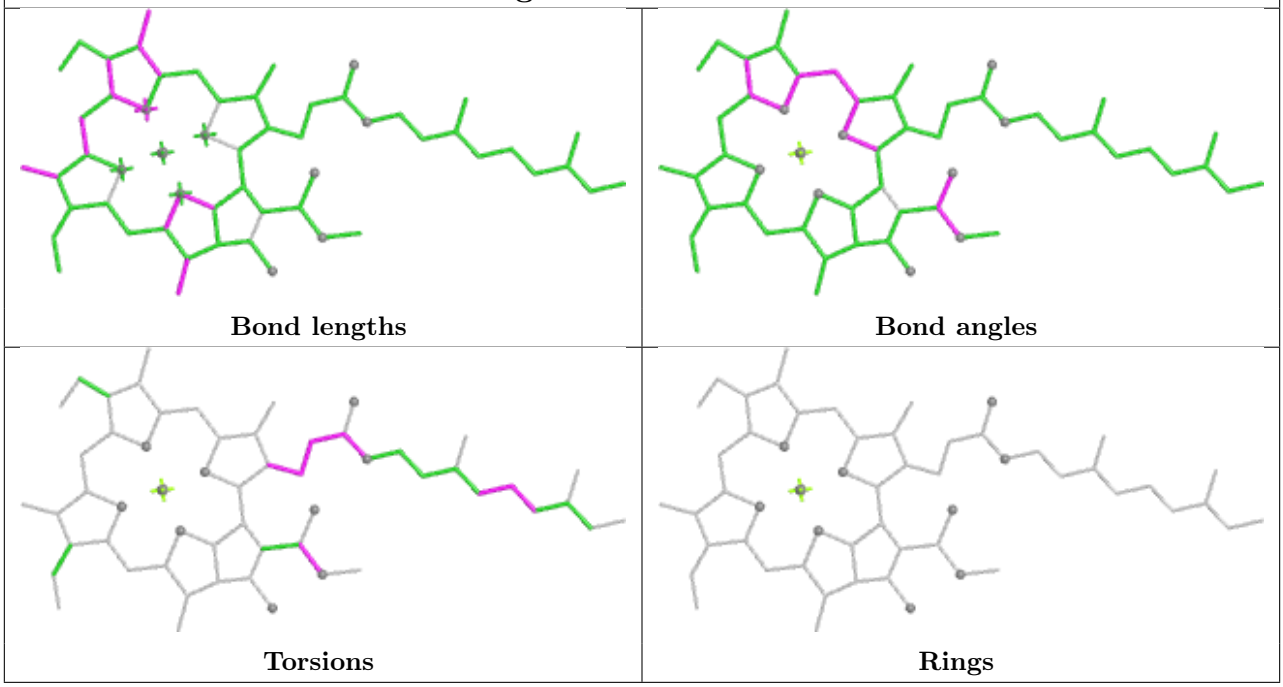


Ligand CLA A6 610



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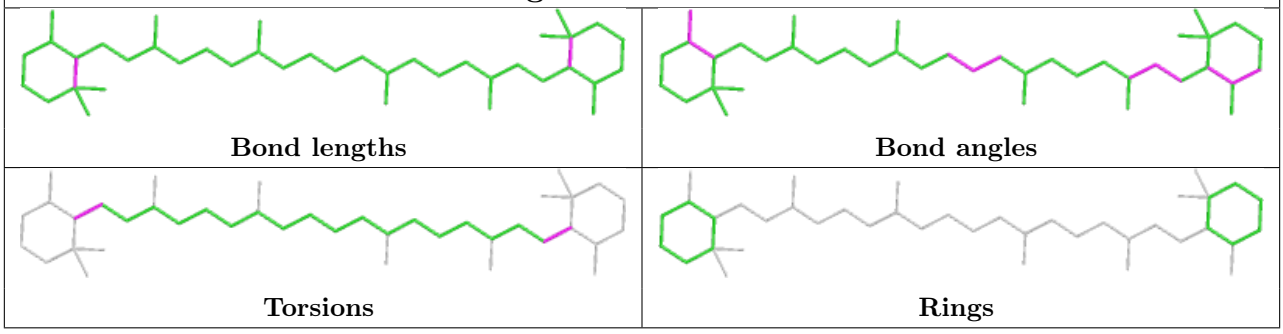

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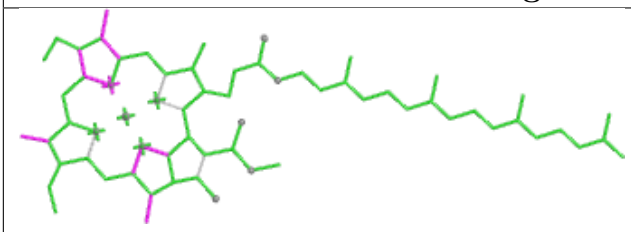
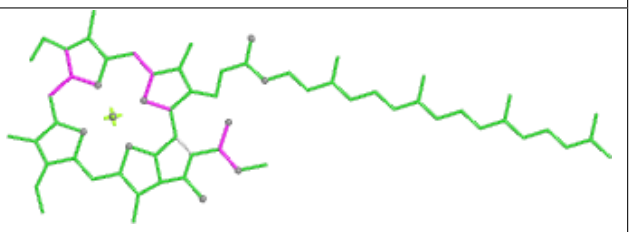
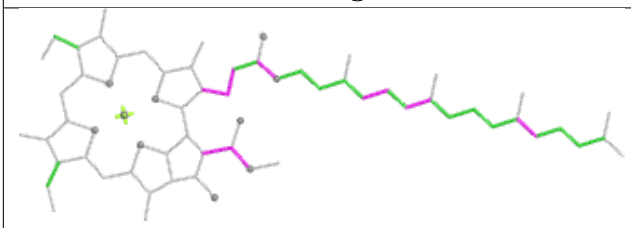


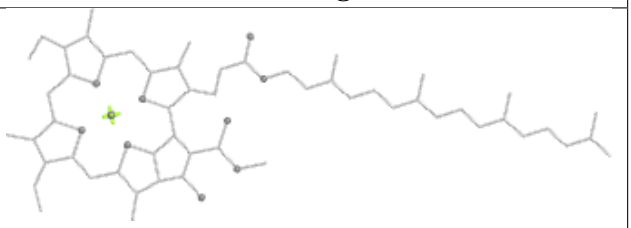
Bond lengths



Bond angles

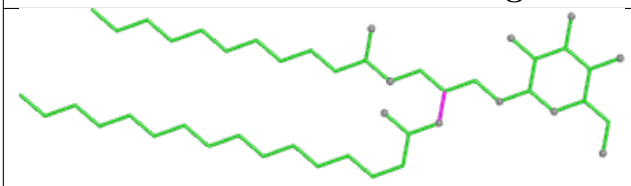


Torsions

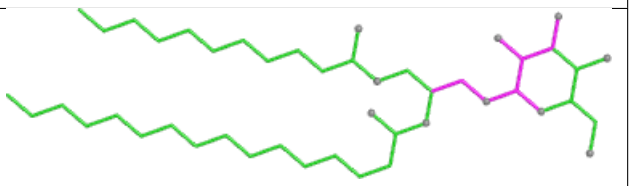


Rings

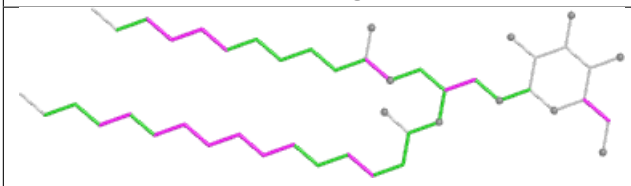
Ligand LMG BG 405



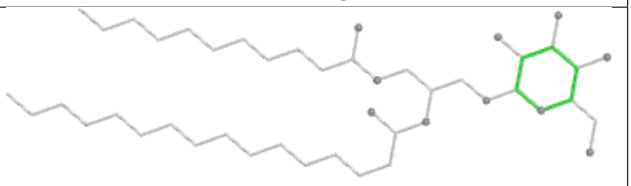
Bond lengths



Bond angles

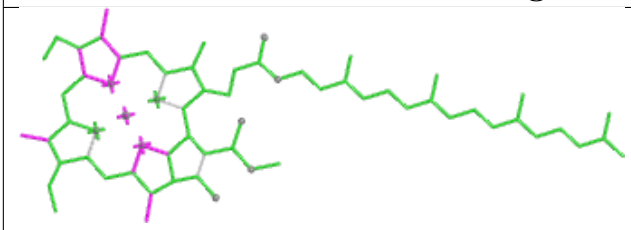


Torsions



Rings

Ligand CLA v 612



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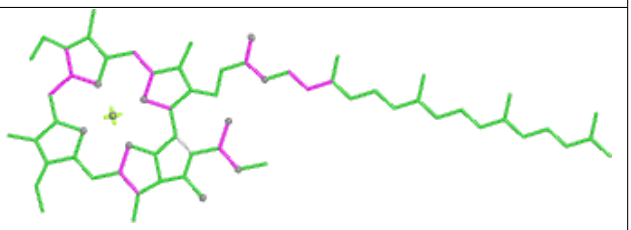
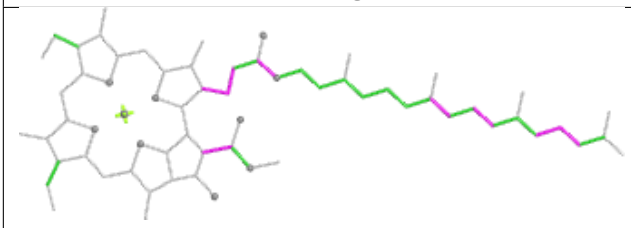


Bond angles



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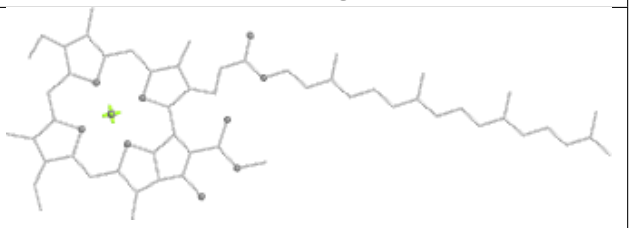
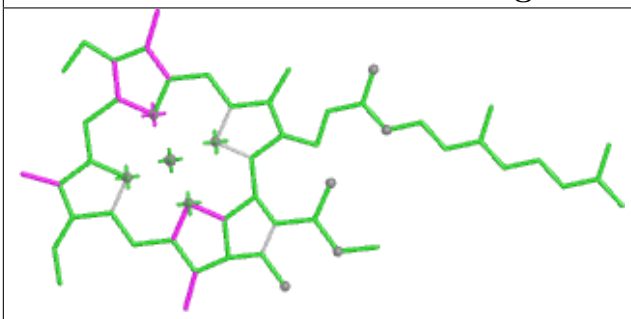
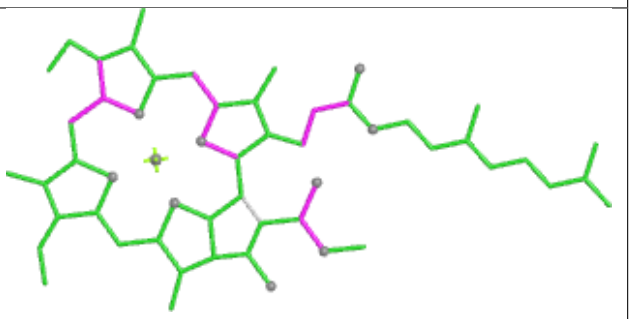
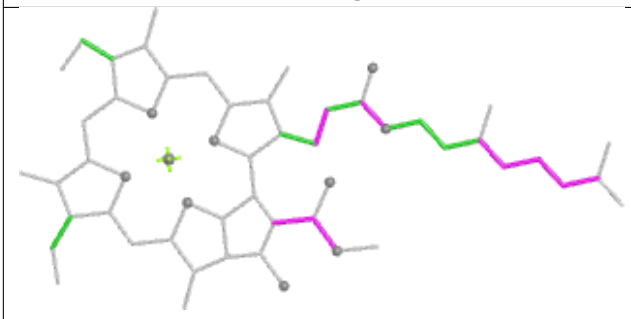
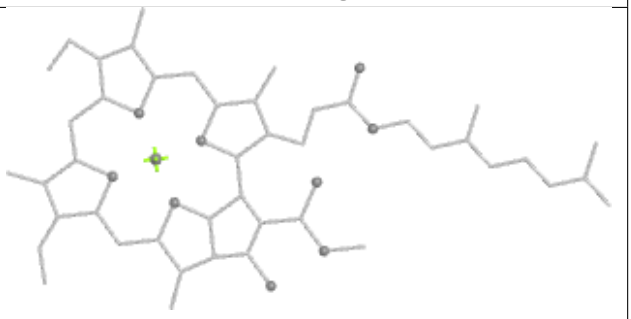
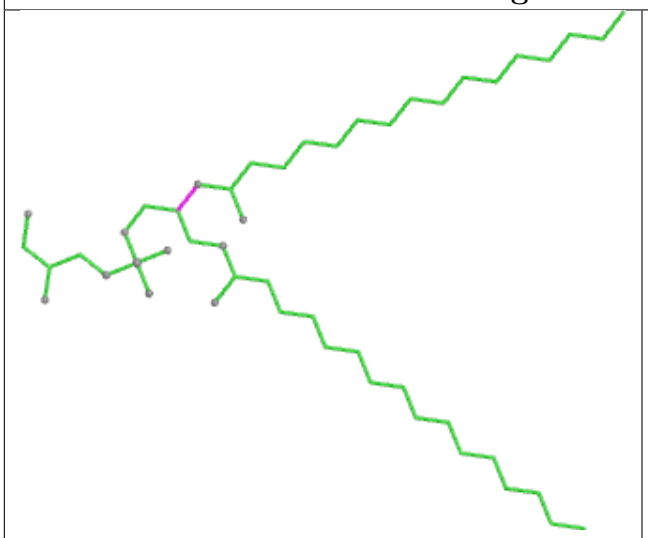


Rings

Ligand CLA A6 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG BB 319



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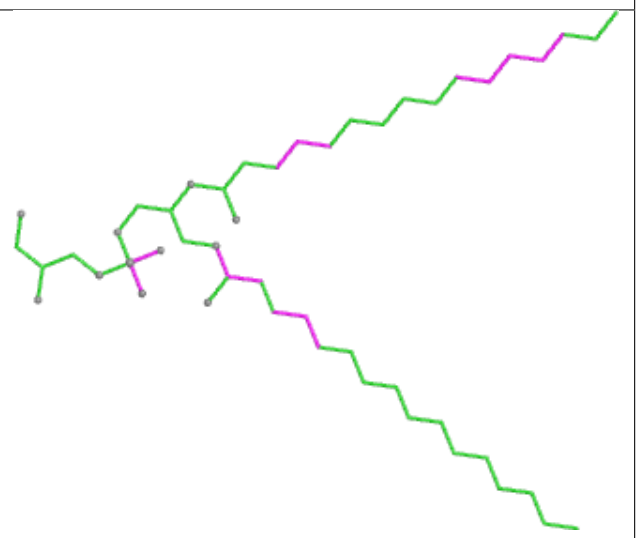
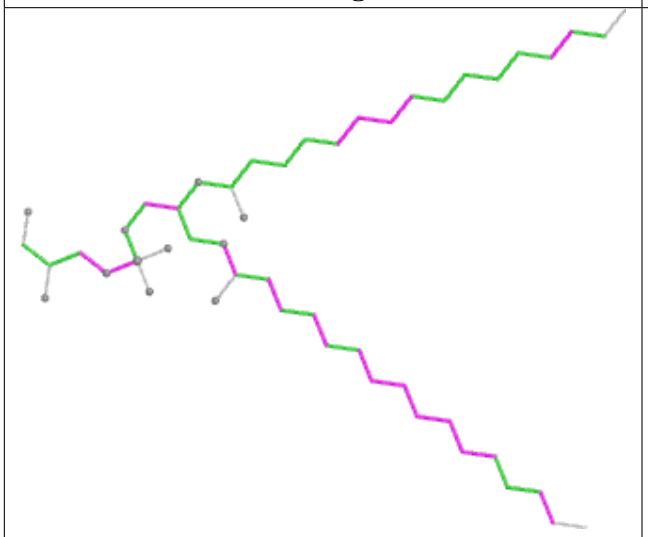


Bond angles



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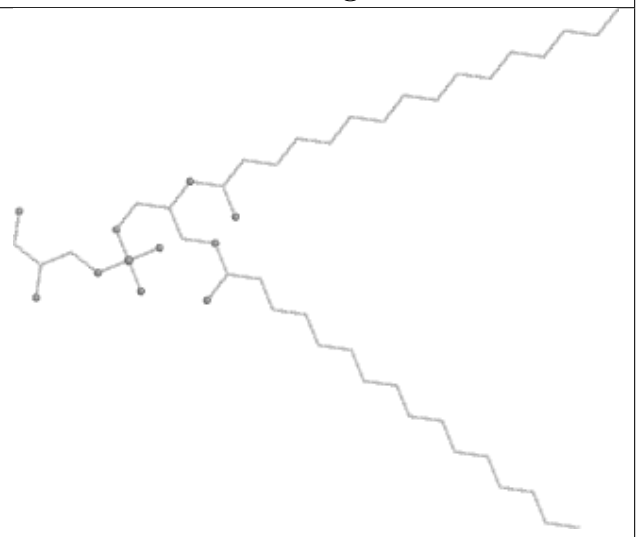
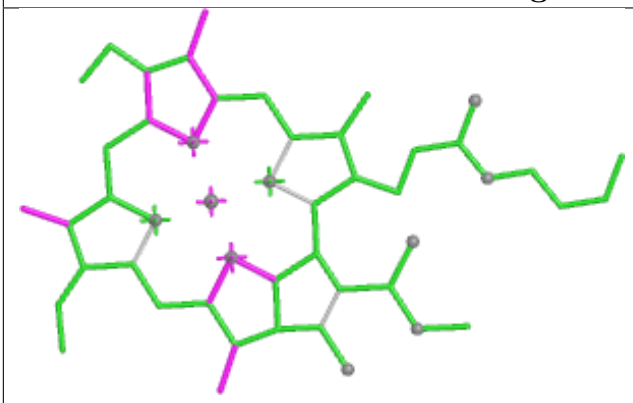


Rings

Ligand CLA r 611



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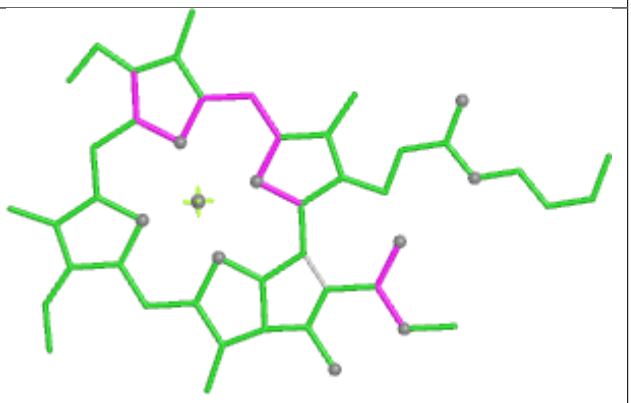
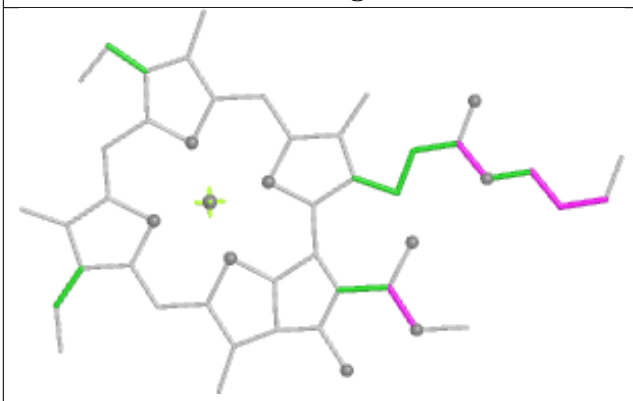


Bond angles



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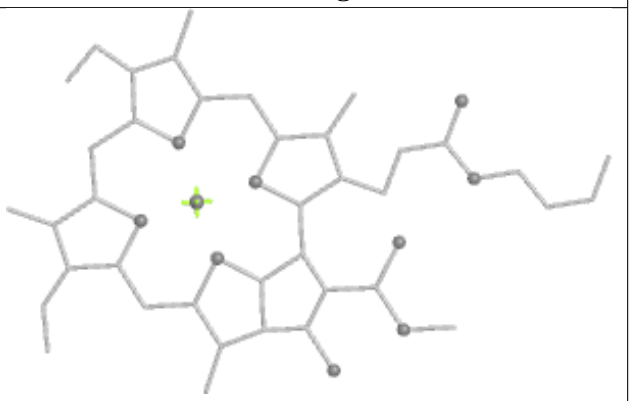
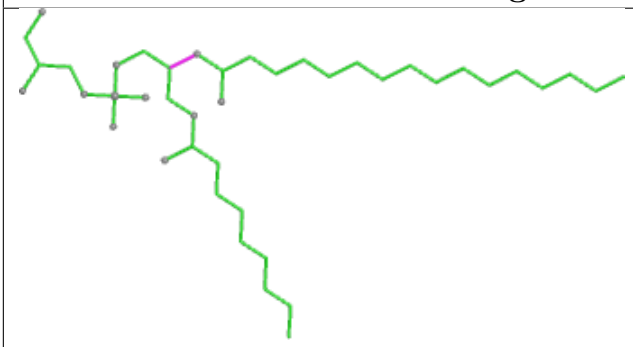


Rings

Ligand LHG BU 617



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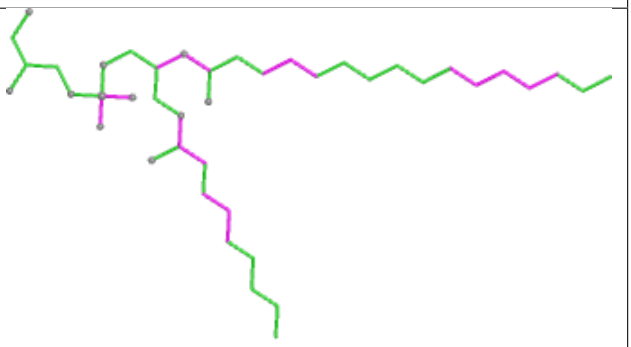
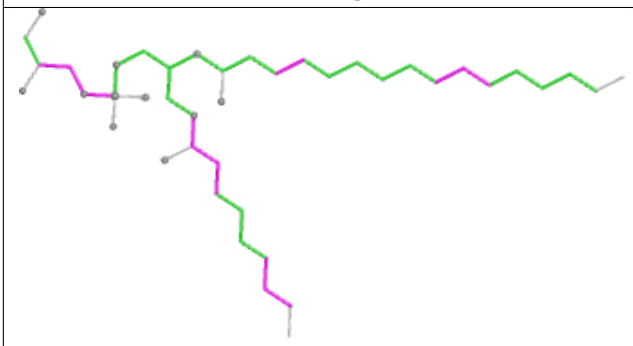


Bond angles



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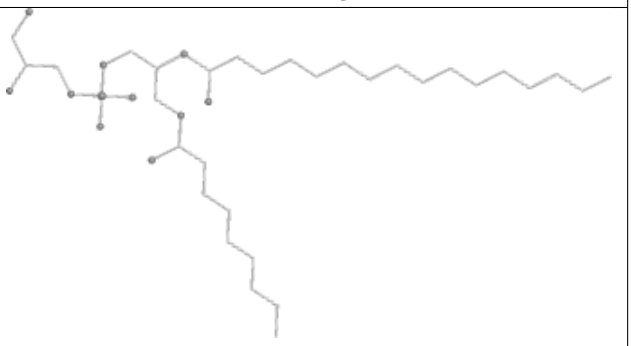
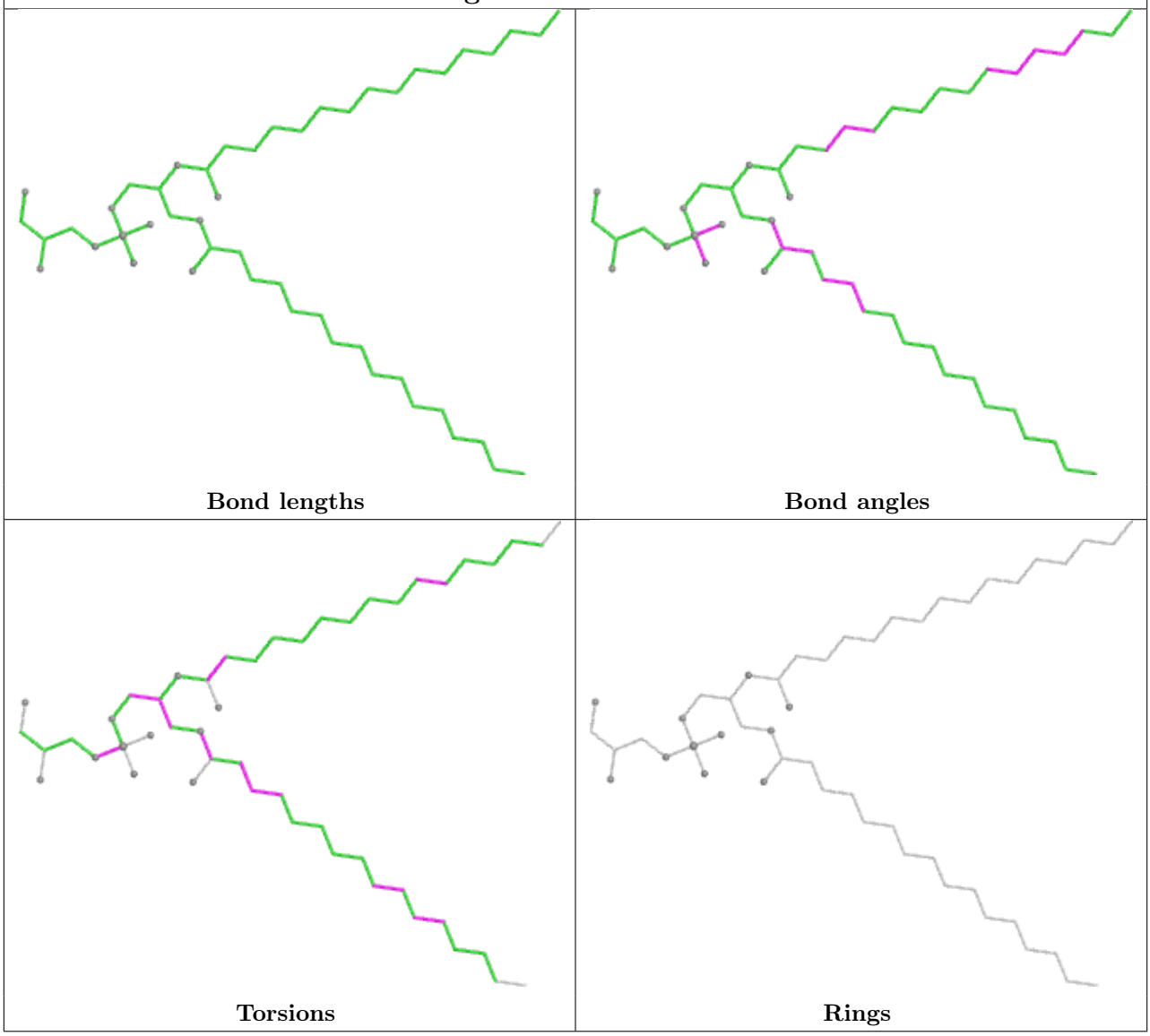
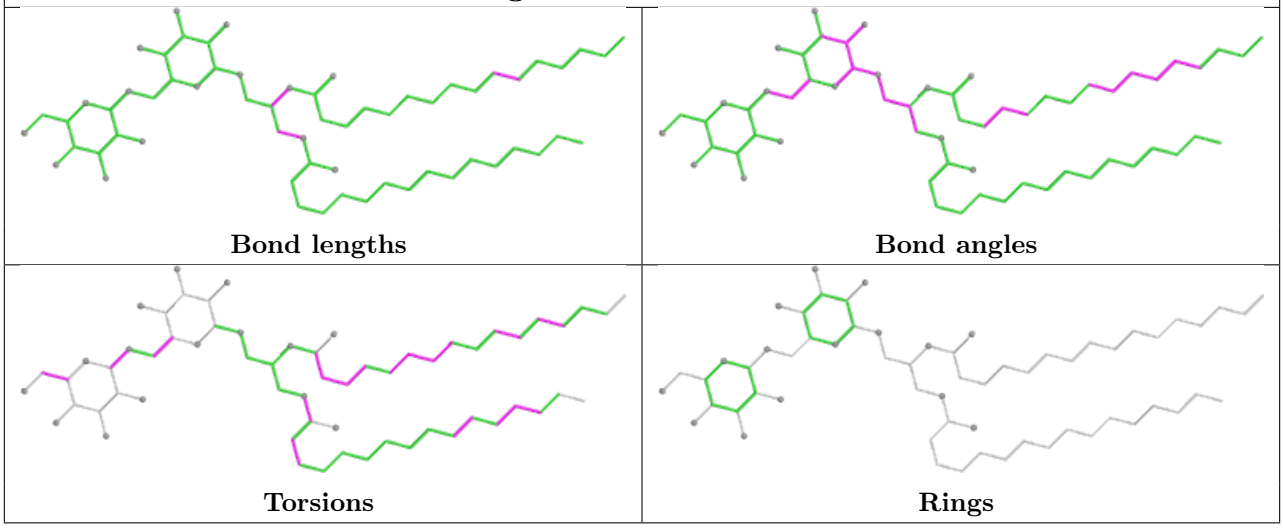


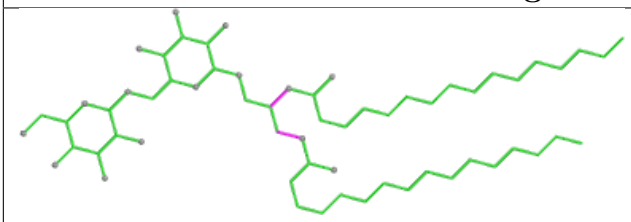
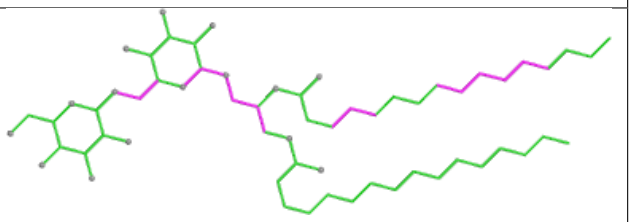
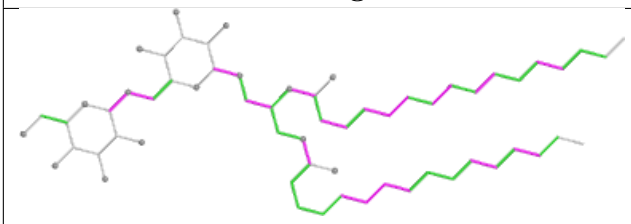
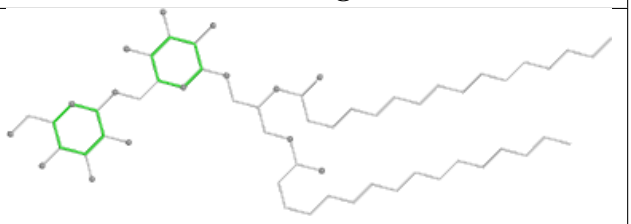
Rings

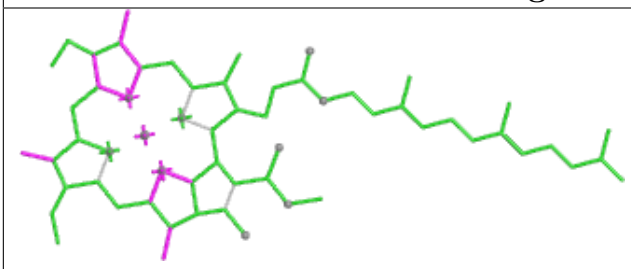
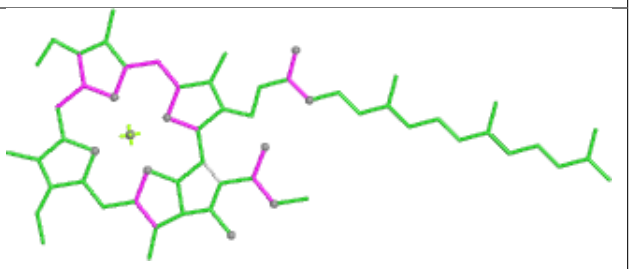
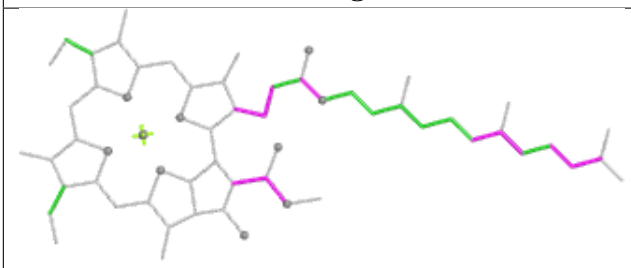
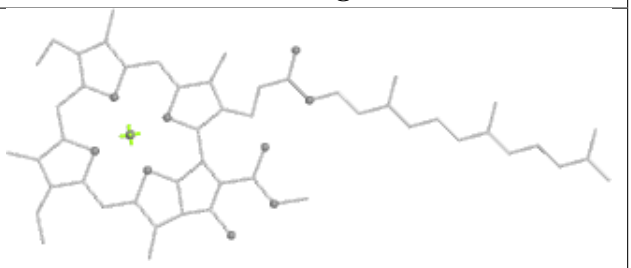
Ligand LHG W 201



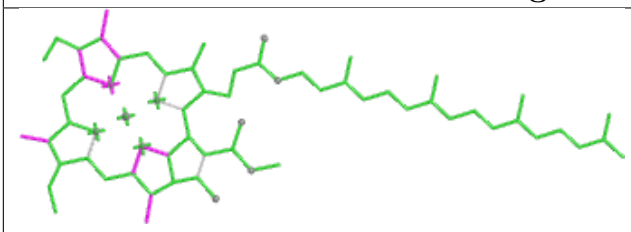
Ligand DGD BK 102



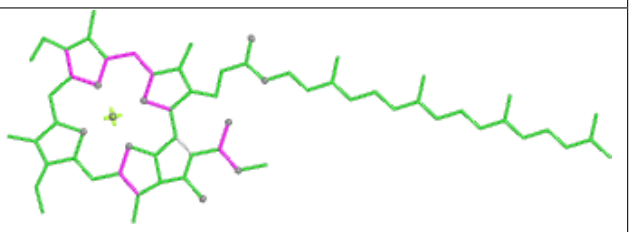
Ligand DGD 1 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

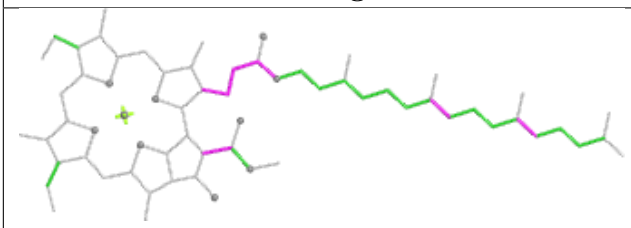
Ligand CLA c 502



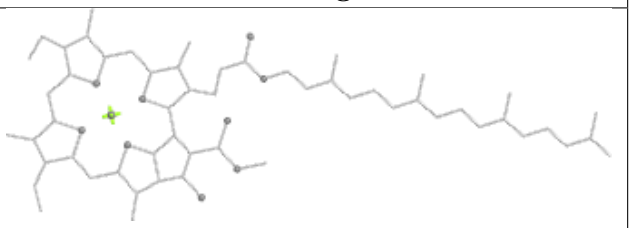
Bond lengths



Bond angles

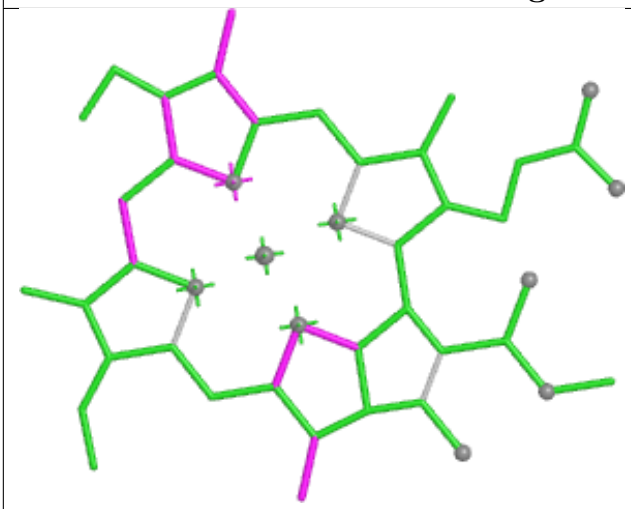


Torsions



Rings

Ligand CLA 7 305



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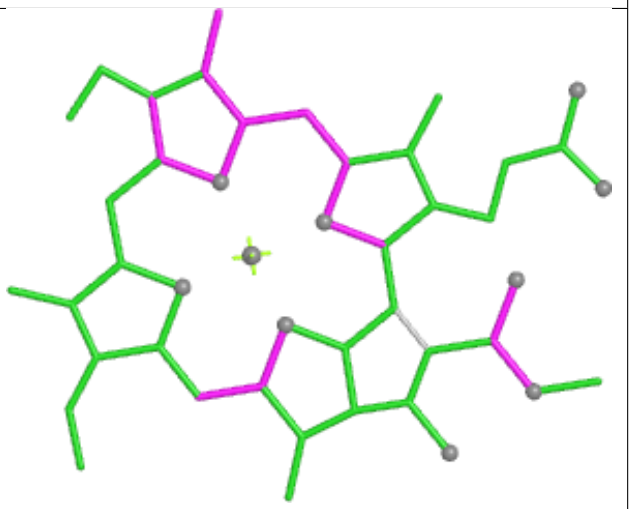
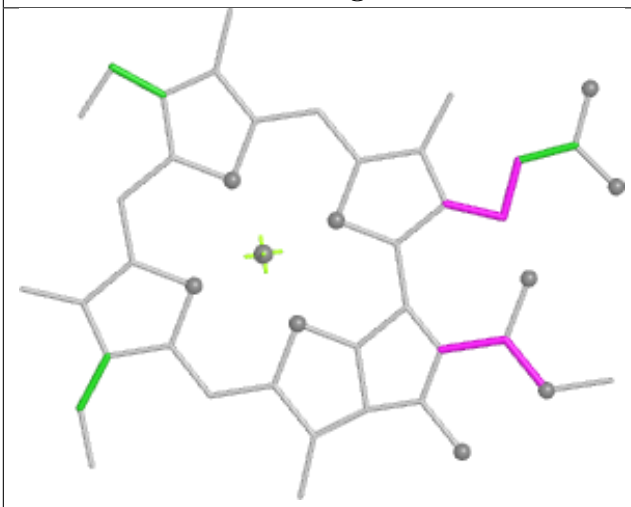


Bond angles



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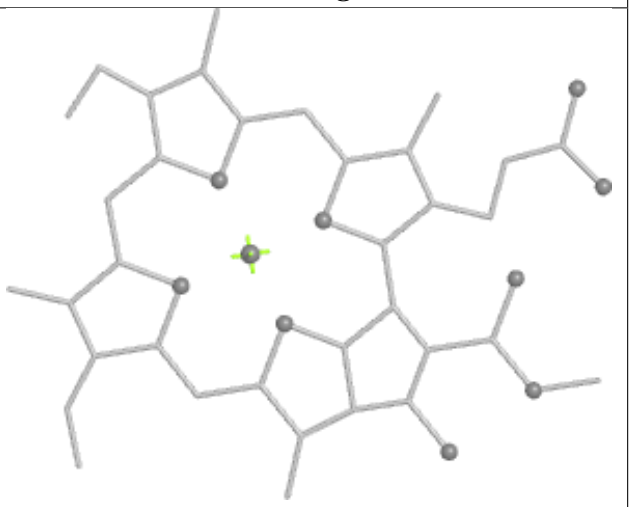
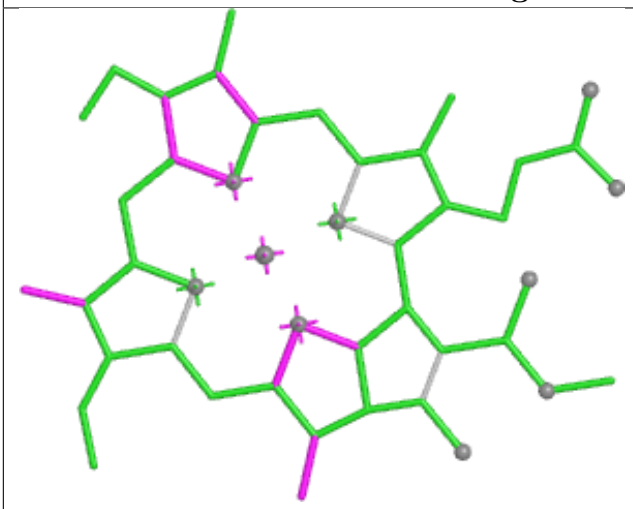


Rings

Ligand CLA AB 303



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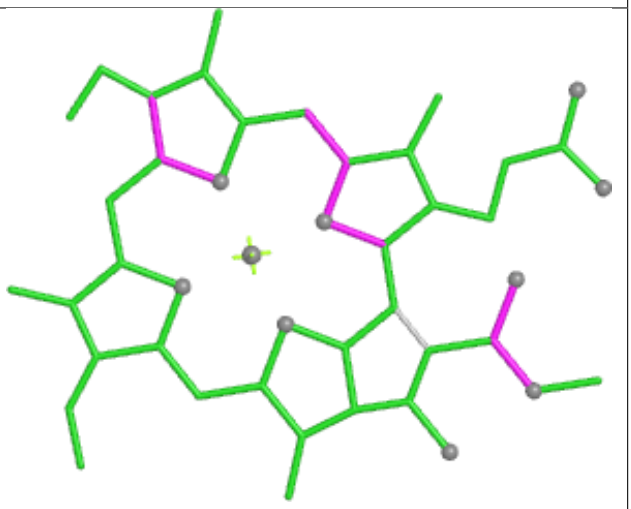
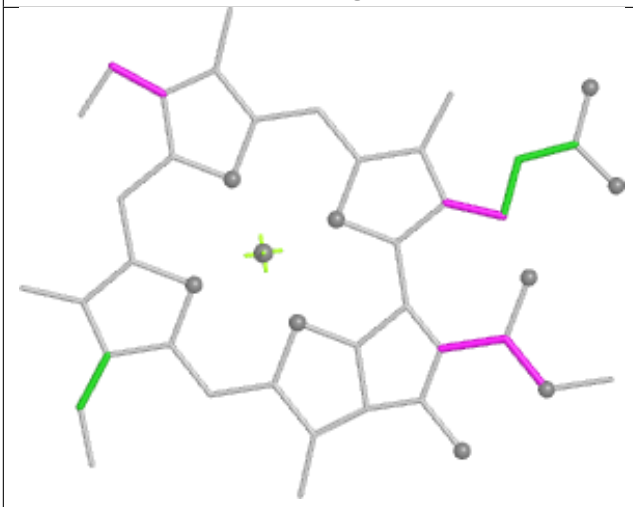


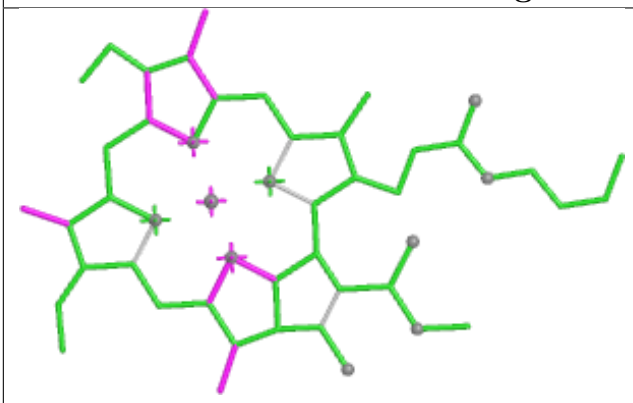
Bond angles



Torsions

Rings

Ligand CLA A6 611



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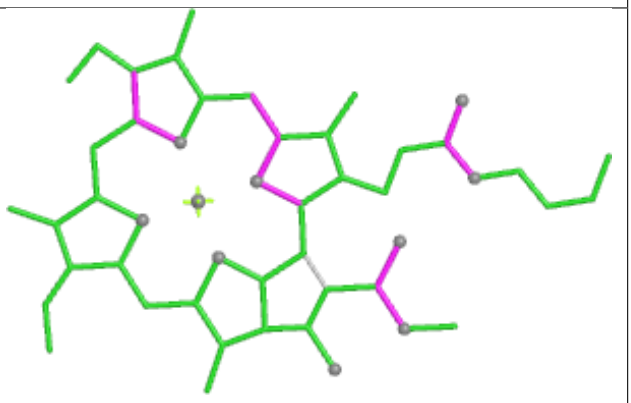

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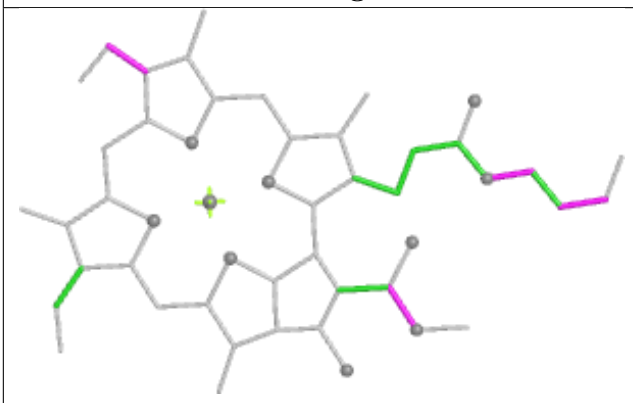

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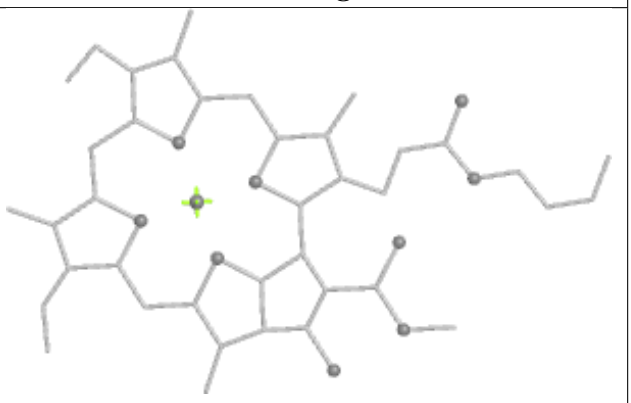
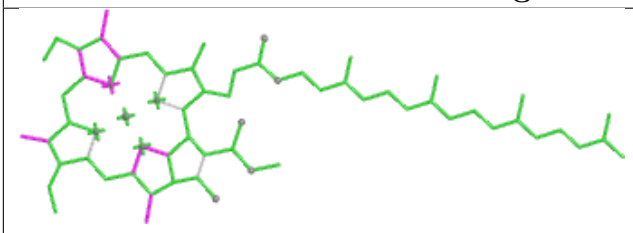


Rings

Ligand CLA BF 502



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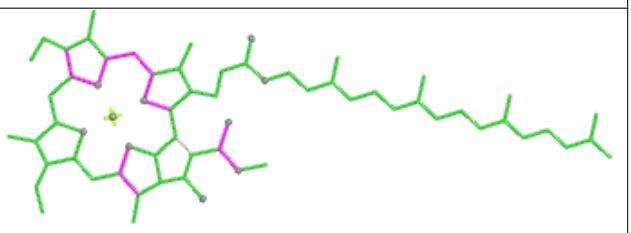

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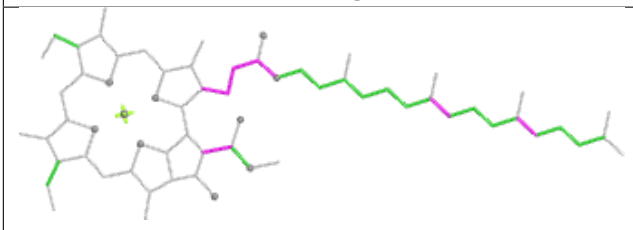

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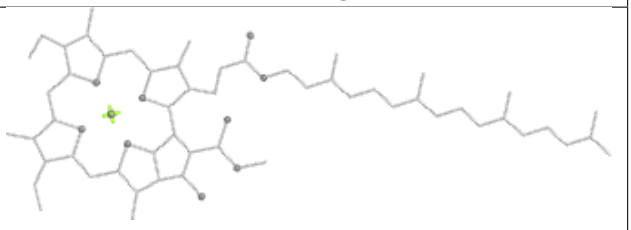
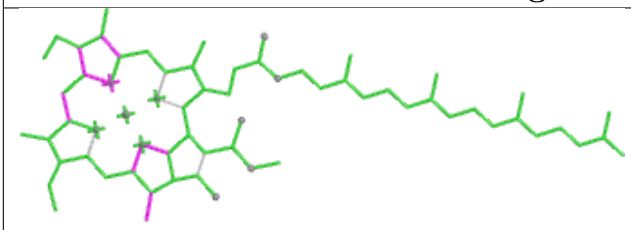


Rings

Ligand CLA g 613



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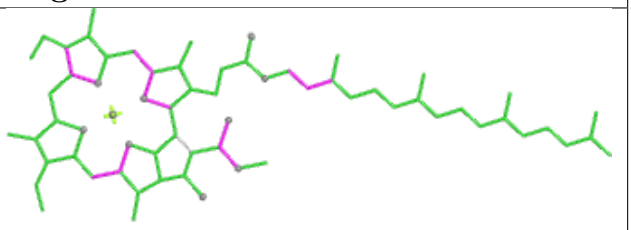
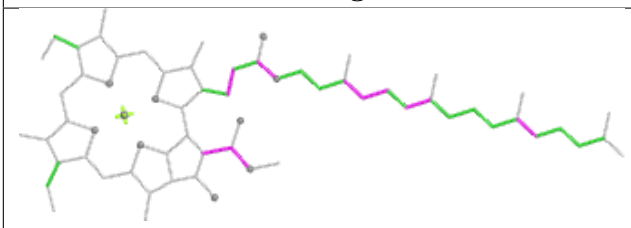


Bond angles



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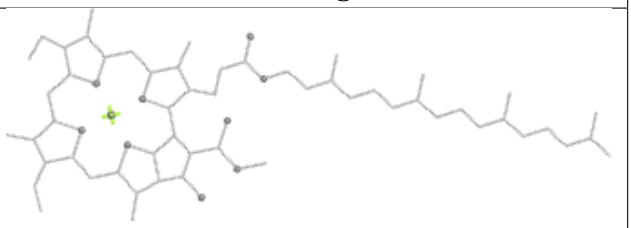
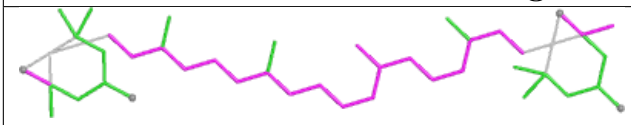
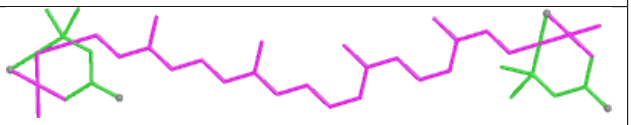


Rings

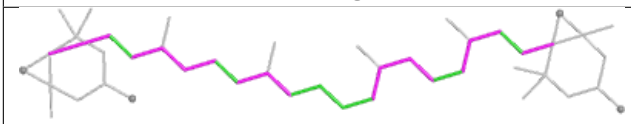
Ligand XAT 7 318



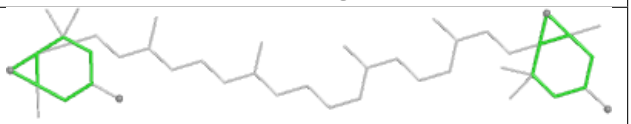
Bond lengths



Bond angles

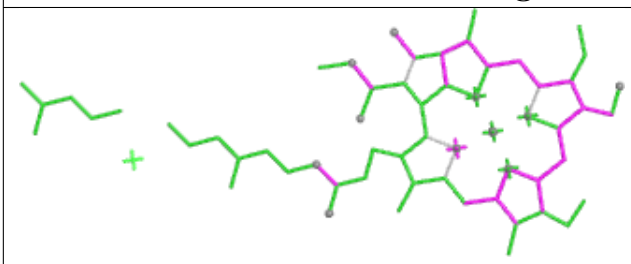


Torsions

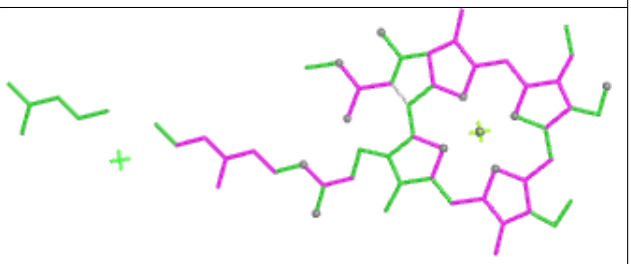


Rings

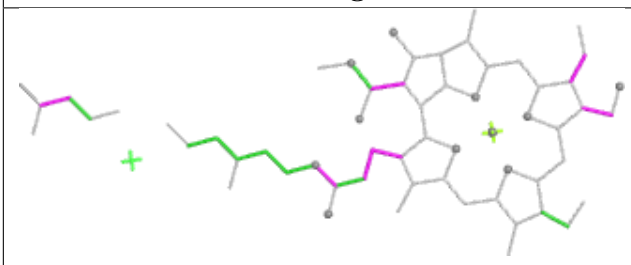
Ligand CHL BJ 609



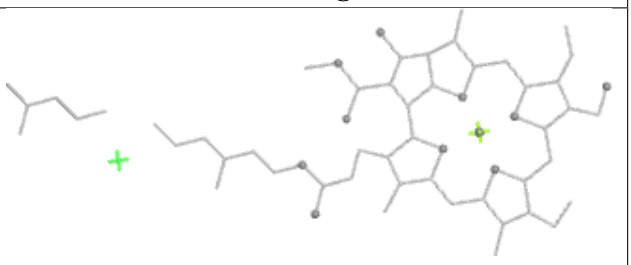
Bond lengths



Bond angles

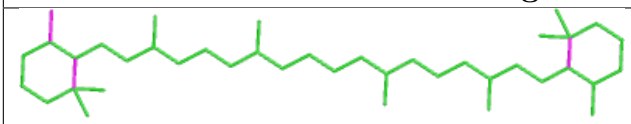


Torsions

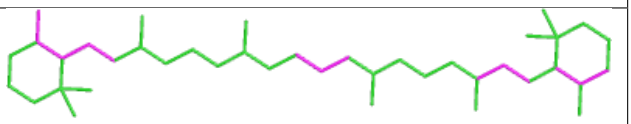


Rings

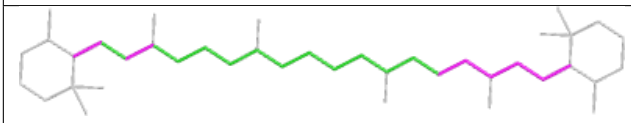
Ligand BCR K 101



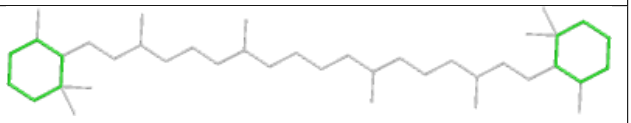
Bond lengths



Bond angles



Torsions

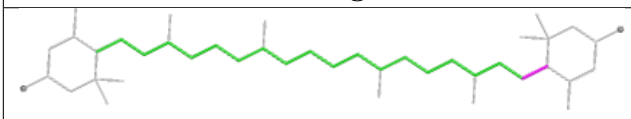


Rings

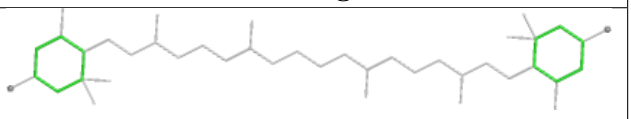
Ligand LUT BQ 615

Bond lengths

Bond angles

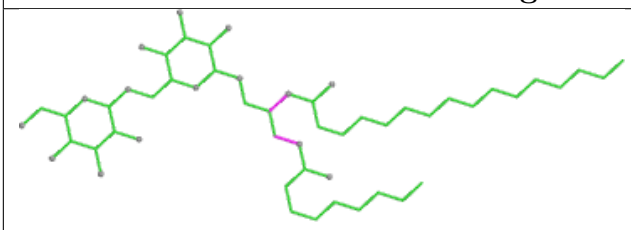


Torsions

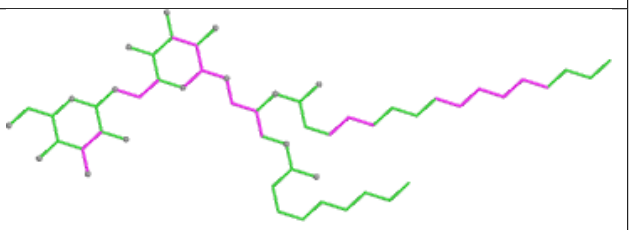


Rings

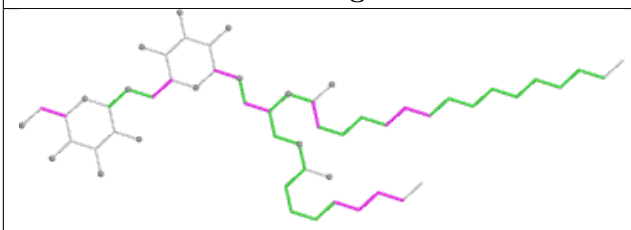
Ligand DGD C 516



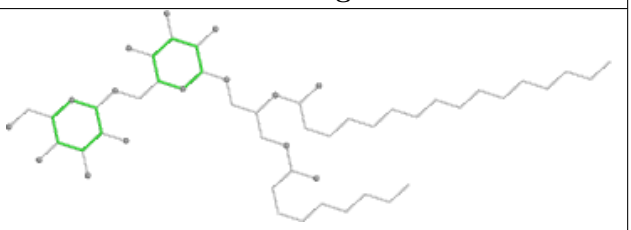
Bond lengths



Bond angles

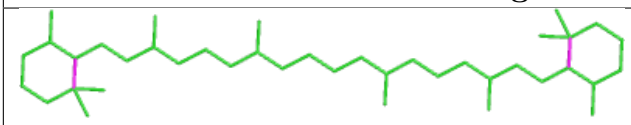


Torsions

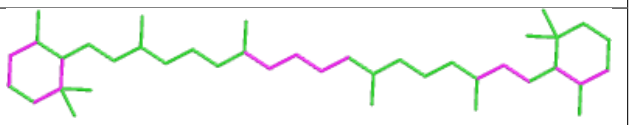


Rings

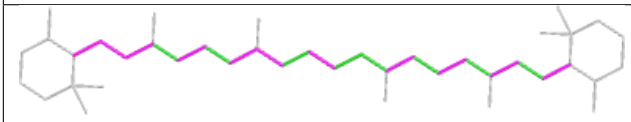
Ligand BCR BE 601



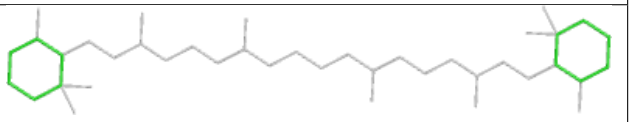
Bond lengths



Bond angles

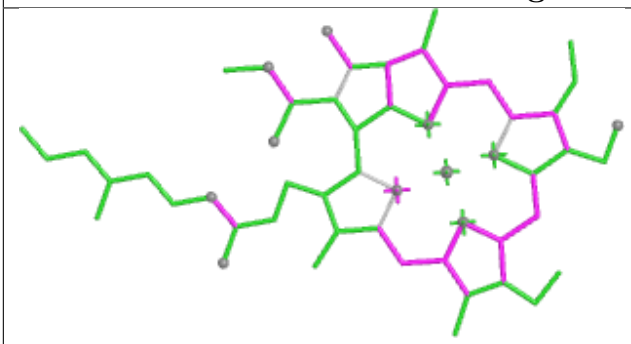


Torsions

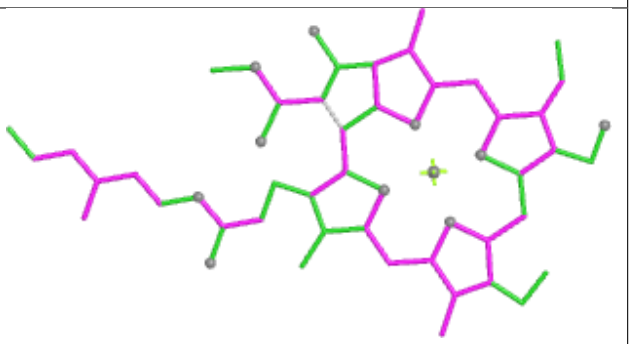


Rings

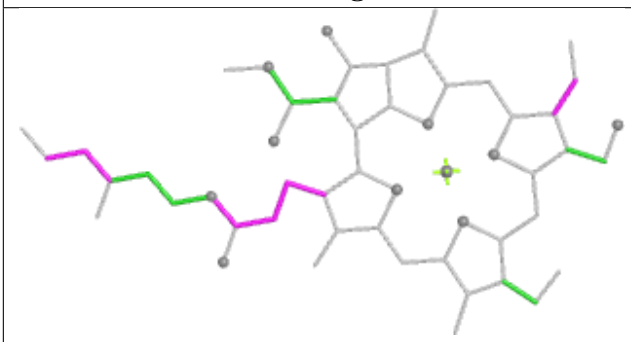
Ligand CHL 6 607



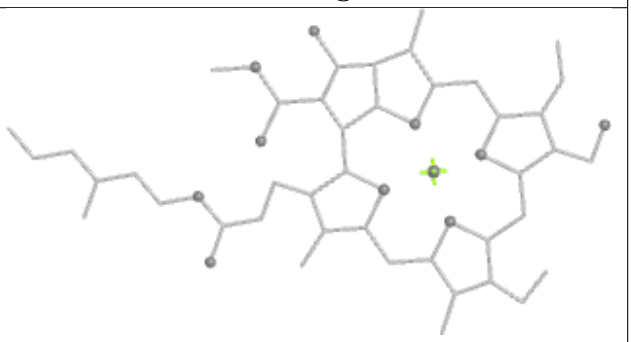
Bond lengths



Bond angles

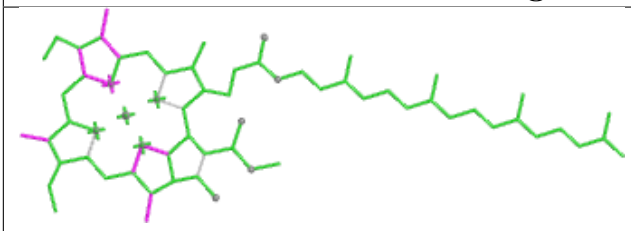


Torsions

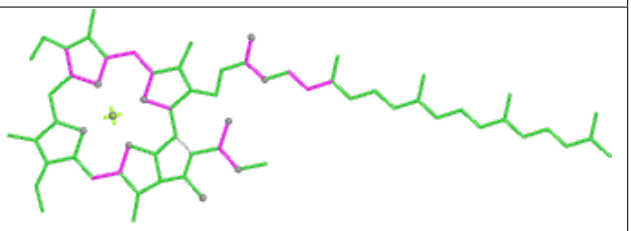


Rings

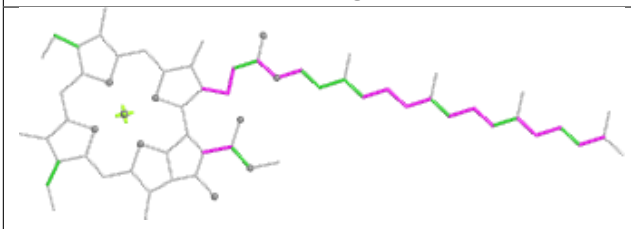
Ligand CLA b 605



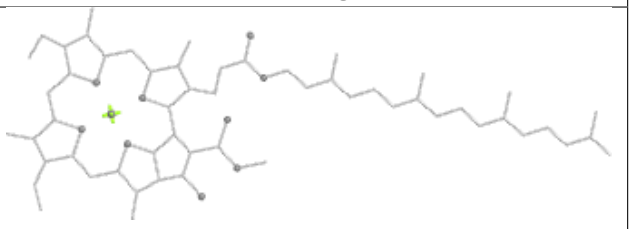
Bond lengths



Bond angles

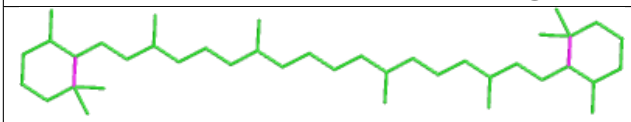


Torsions

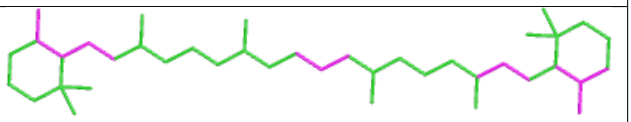


Rings

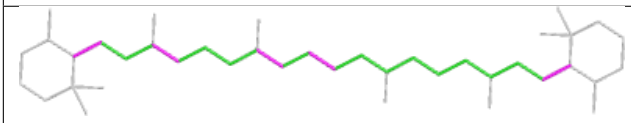
Ligand BCR v 619



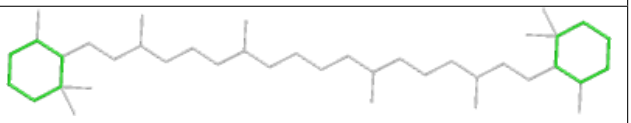
Bond lengths



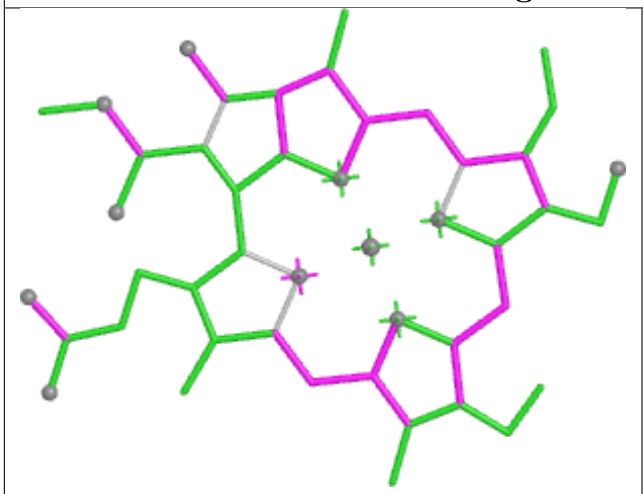
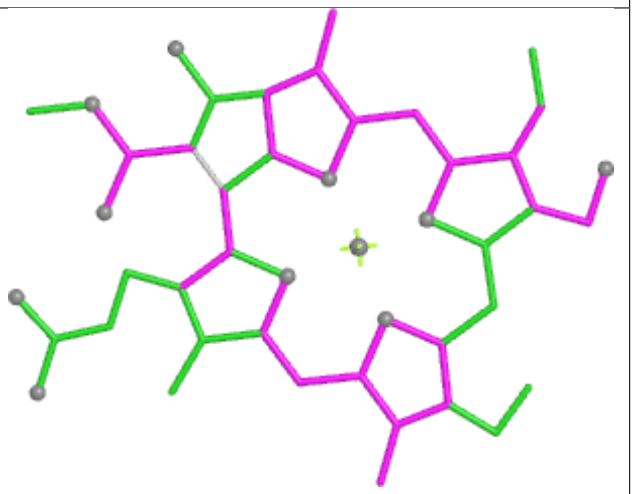
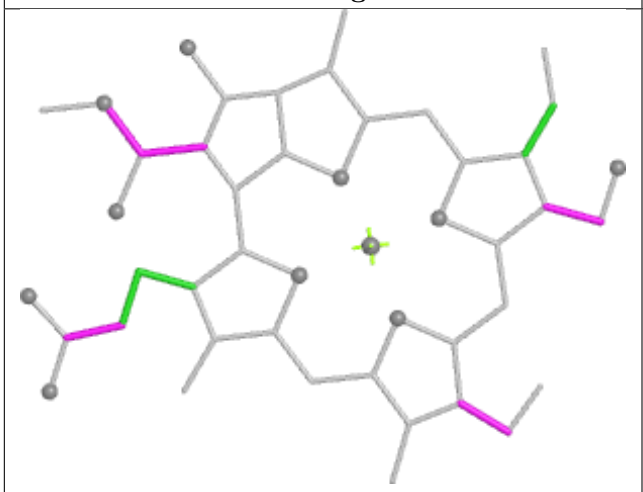
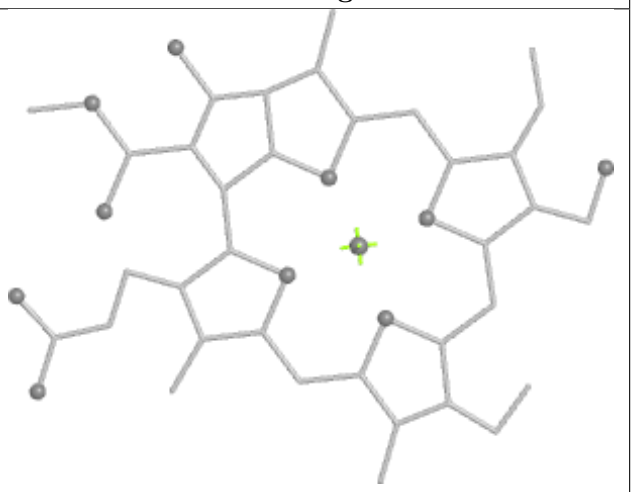
Bond angles



Torsions



Rings

Ligand CHL A6 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

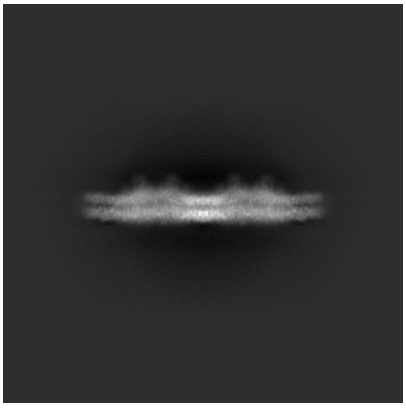
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-63017. These allow visual inspection of the internal detail of the map and identification of artifacts.

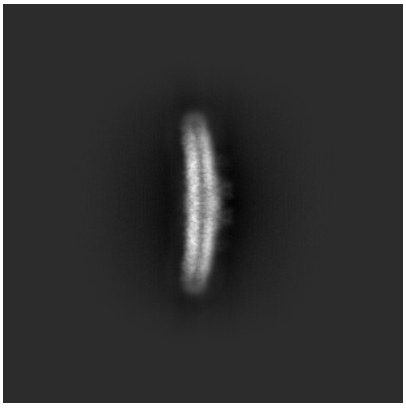
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

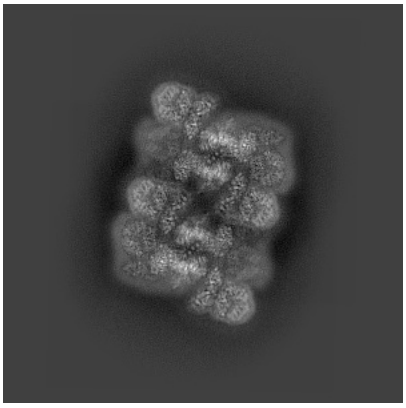
6.1.1 Primary map



X



Y

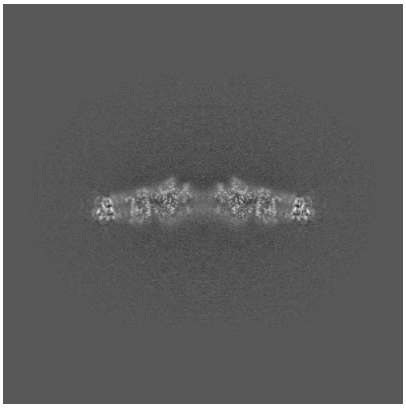


Z

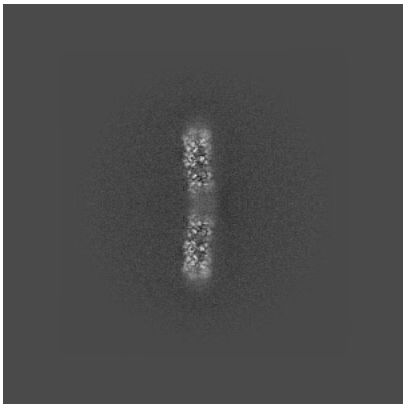
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

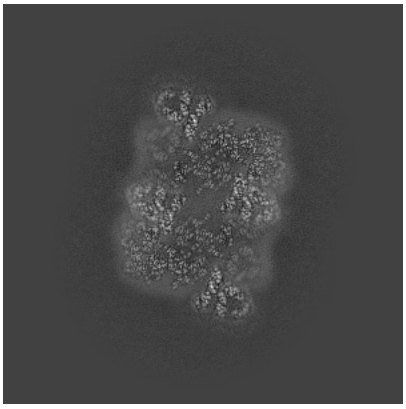
6.2.1 Primary map



X Index: 360



Y Index: 360

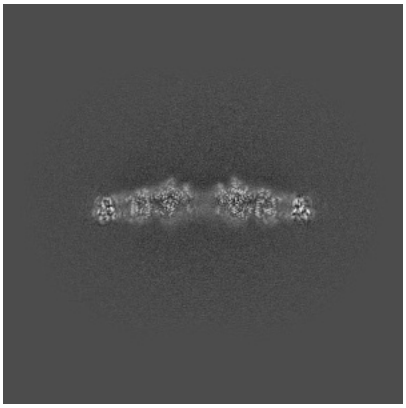


Z Index: 360

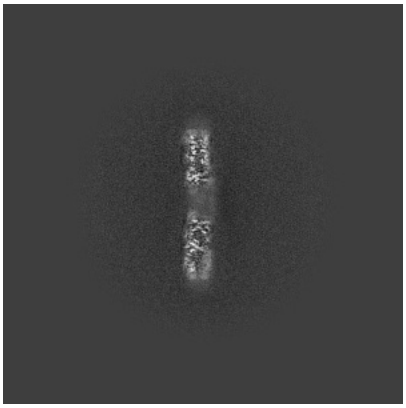
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

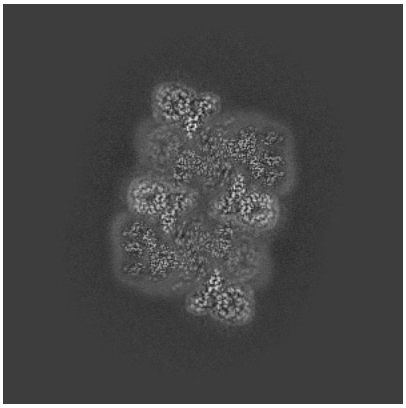
6.3.1 Primary map



X Index: 361



Y Index: 367

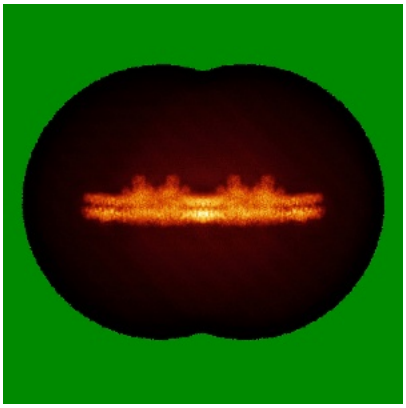


Z Index: 342

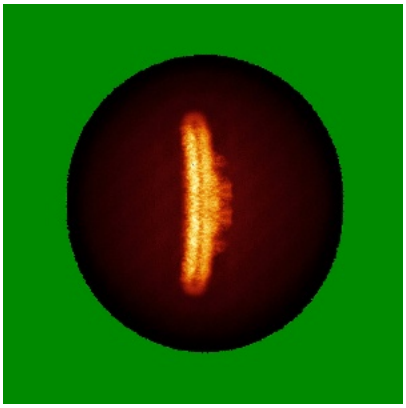
The images above show the largest variance slices of the map in three orthogonal directions.

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

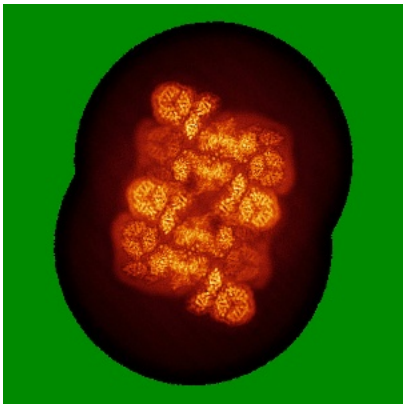
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

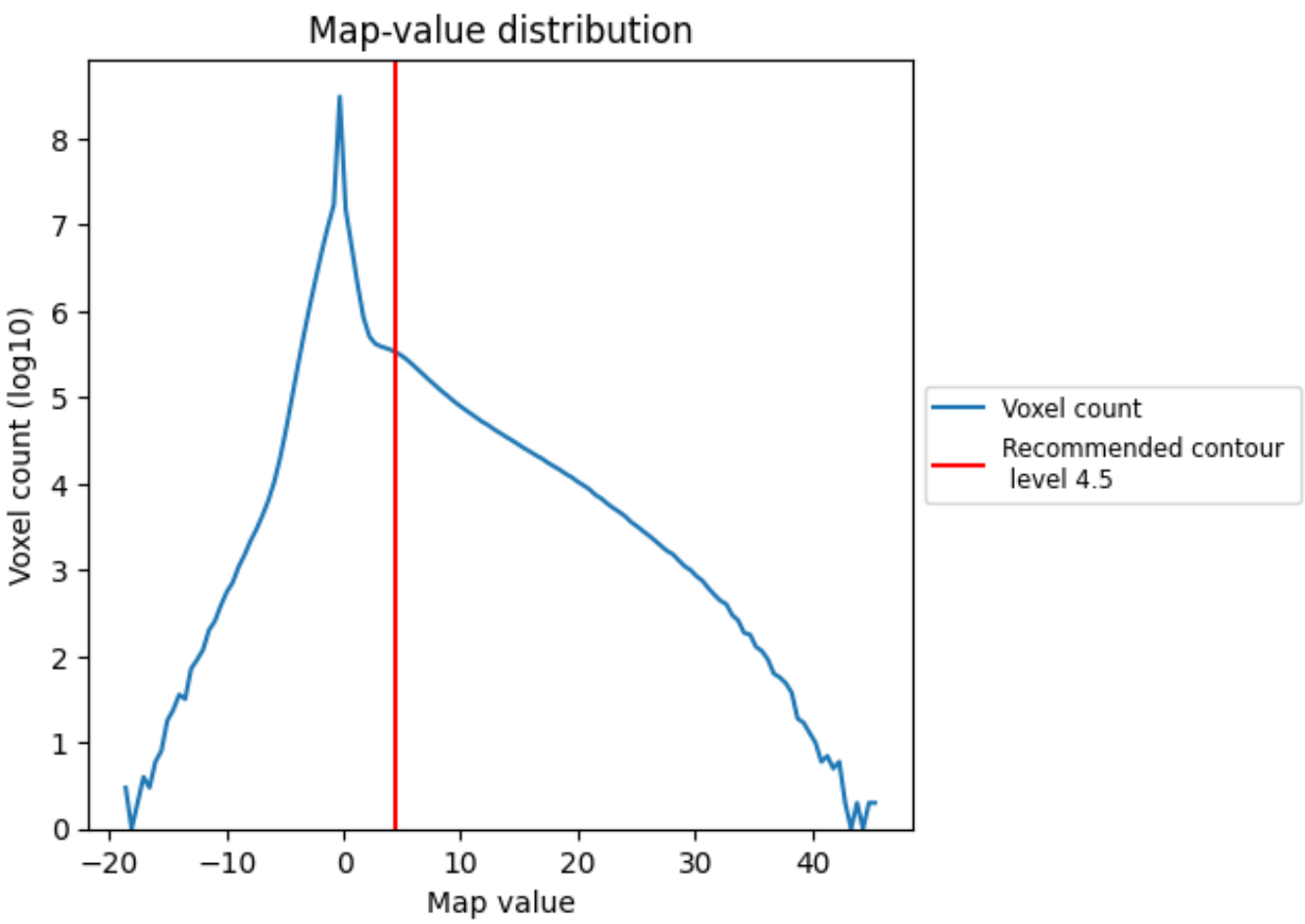
6.6 Mask visualisation (i)

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

7 Map analysis (i)

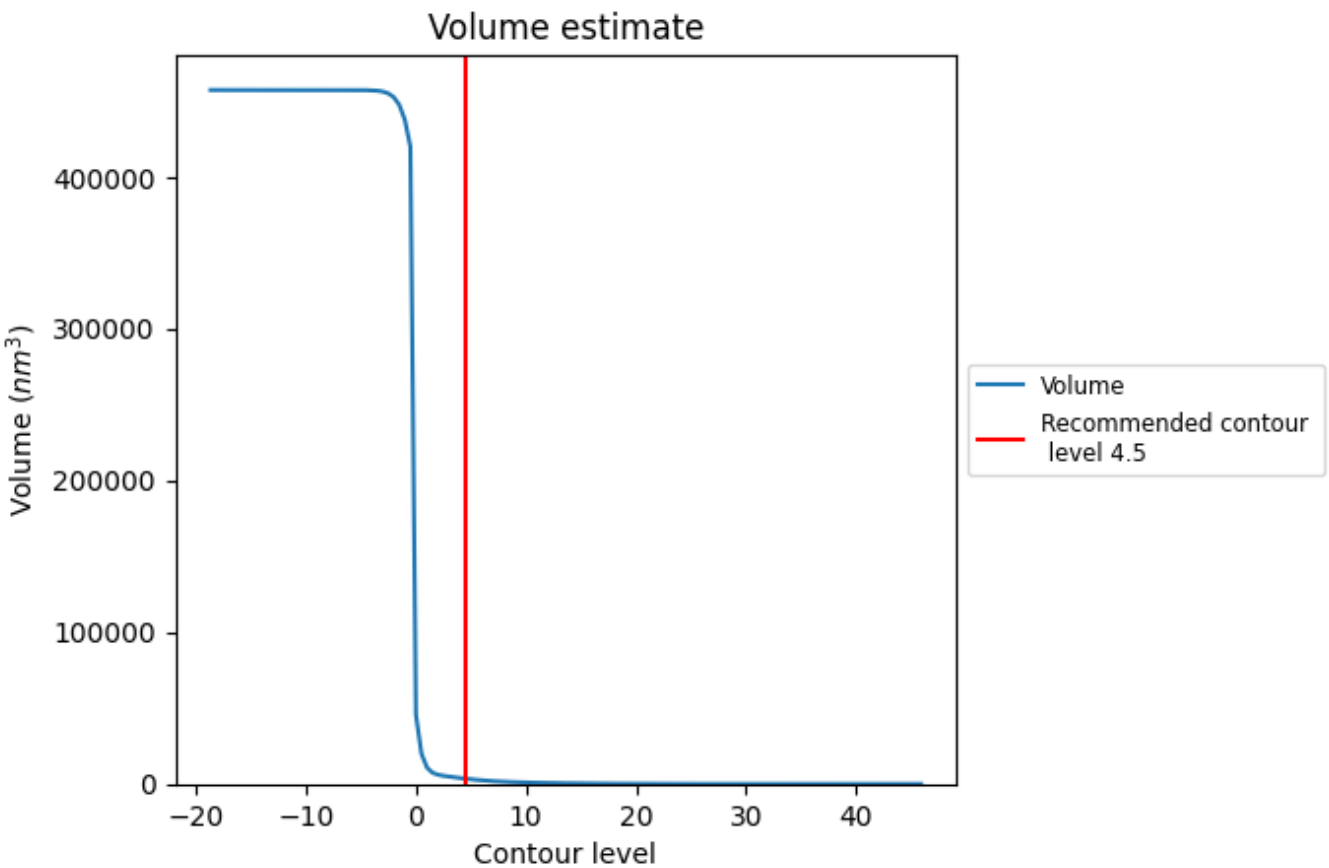
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

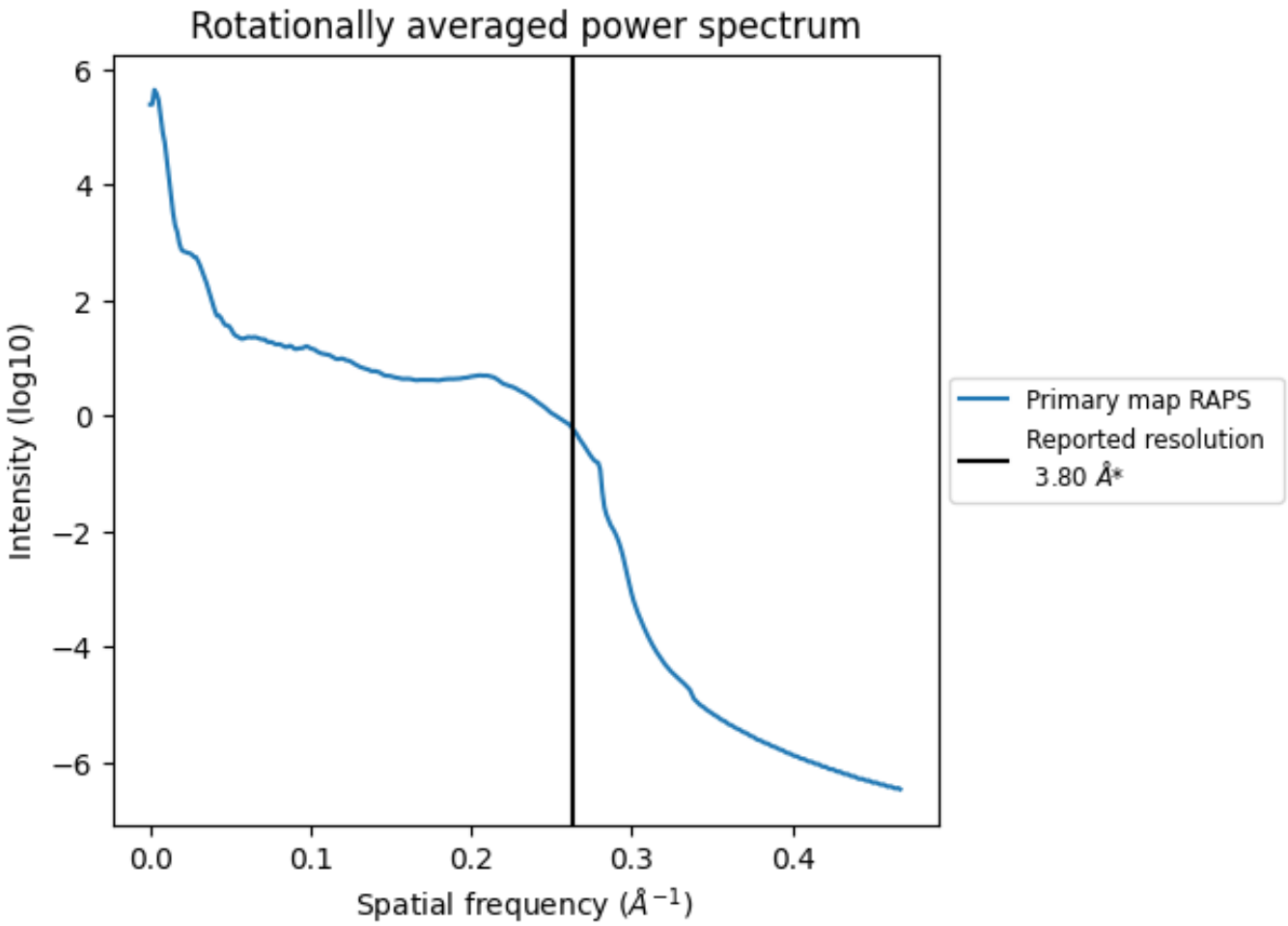
7.2 Volume estimate (i)



The volume at the recommended contour level is 3500 nm^3; this corresponds to an approximate mass of 3162 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 0.263 Å^{-1}

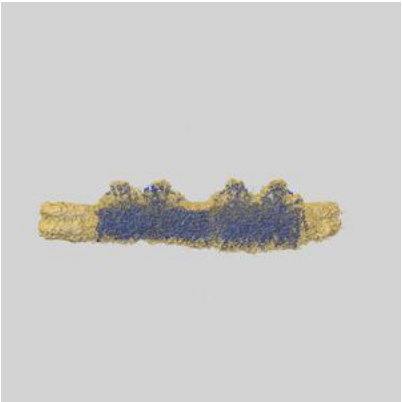
8 Fourier-Shell correlation (i)

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

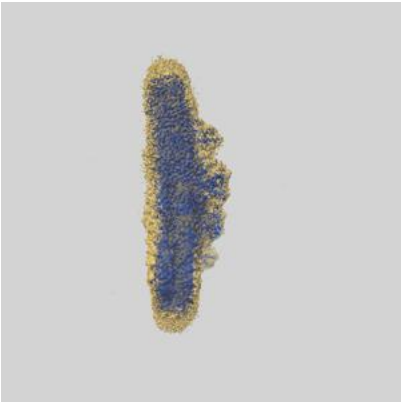
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-63017 and PDB model 9LE7. Per-residue inclusion information can be found in section 3 on page 58.

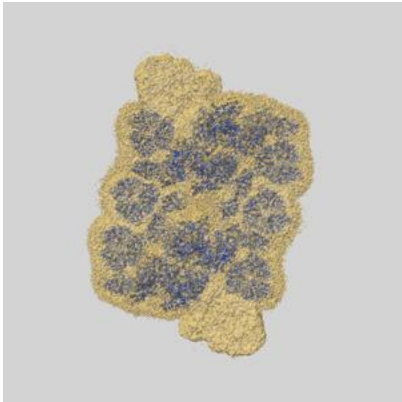
9.1 Map-model overlay (i)



X



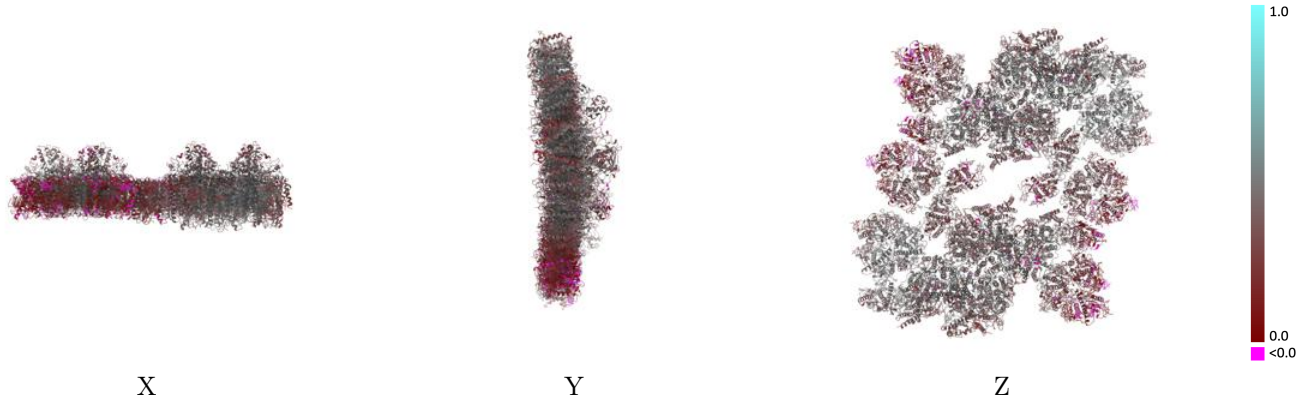
Y



Z

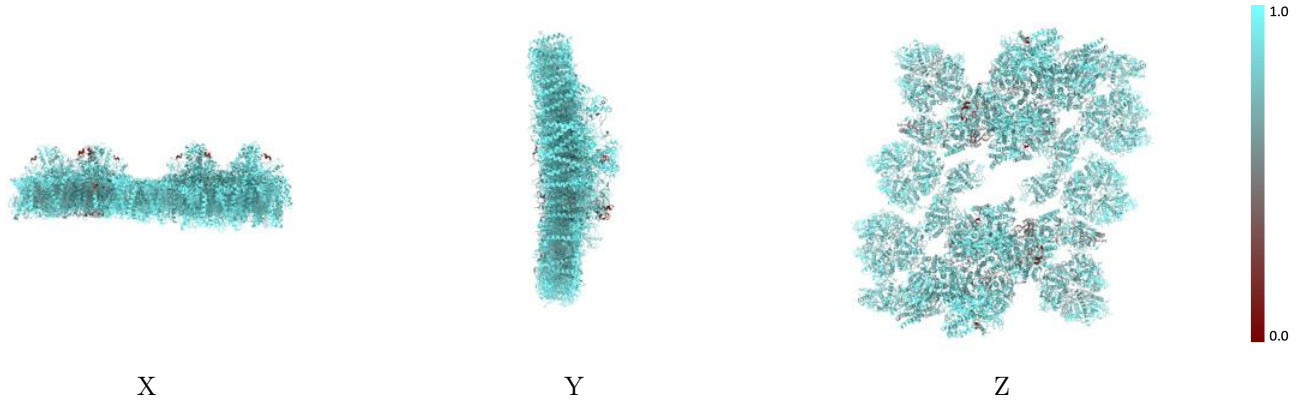
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



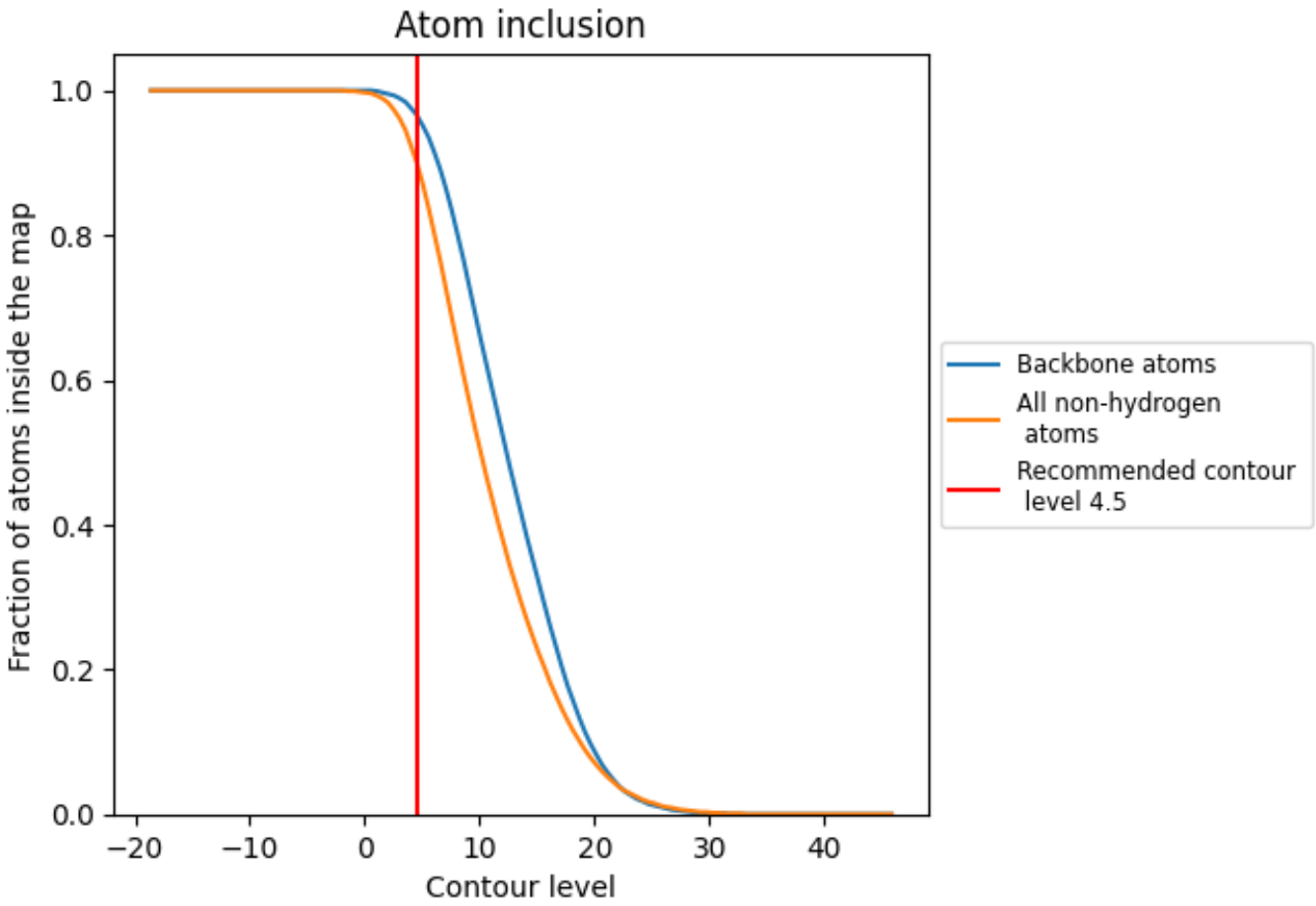
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.3560
0	0.9480	0.3160
1	0.9370	0.4360
2	0.9520	0.4400
3	0.9320	0.3050
4	0.8930	0.3100
5	0.9690	0.2760
6	0.9510	0.3040
7	0.9720	0.1710
8	0.9130	0.2480
9	0.9670	0.2830
A	0.9210	0.4230
A0	0.8670	0.3990
A1	0.8980	0.3770
A2	0.9450	0.4500
A6	0.8890	0.4040
A7	0.8350	0.4330
A8	0.6400	0.2120
AA	0.9690	0.1720
AB	0.9110	0.2560
Au	0.9410	0.3990
Av	0.9380	0.3490
Aw	0.9420	0.4570
Ay	0.9050	0.4320
Az	0.8940	0.4450
B	0.9210	0.4060
BA	0.8270	0.2090
BB	0.9290	0.4590
BC	0.8680	0.3250
BD	0.9040	0.4230
BE	0.9140	0.3960
BF	0.8370	0.4210
BG	0.9130	0.4230
BH	0.9210	0.2950
BI	0.8260	0.3230

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Chain	Atom inclusion	Q-score
BJ	0.8500	0.1420
BK	0.8970	0.3390
BL	0.8870	0.4330
BN	0.8080	0.3960
BO	0.9110	0.4230
BP	0.9160	0.3920
BQ	0.8550	0.1890
BU	0.9390	0.3370
BV	0.7600	0.2290
BW	0.8640	0.4060
BX	0.7990	0.2080
BY	0.8310	0.3500
BZ	0.7580	0.2340
Ba	0.8710	0.3090
Bb	0.9200	0.3420
C	0.9310	0.4240
D	0.9480	0.4270
E	0.9320	0.2950
F	0.8800	0.2980
G	0.9380	0.3880
H	0.9210	0.3270
I	0.9320	0.4500
K	0.8860	0.4190
L	0.8960	0.4270
M	0.8550	0.3610
N	0.9350	0.4410
R	0.9280	0.4320
S	0.8790	0.3960
T	0.8390	0.4080
U	0.6450	0.2100
W	0.8690	0.3810
X	0.8270	0.2140
Y	0.9250	0.4470
Z	0.8600	0.3170
a	0.8980	0.4140
b	0.9080	0.3850
c	0.8280	0.4060
d	0.9010	0.4090
e	0.9230	0.2840
f	0.8130	0.3050
g	0.8530	0.1340
h	0.8620	0.3220

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Chain	Atom inclusion	Q-score
i	0.8690	0.4210
k	0.7780	0.3800
l	0.8880	0.4130
m	0.9080	0.3870
n	0.8570	0.1790
r	0.9370	0.3280
s	0.7480	0.2090
t	0.8520	0.3960
u	0.8040	0.2000
v	0.9260	0.4160
w	0.8310	0.3380
x	0.7420	0.2240
y	0.8680	0.2970
z	0.9120	0.3420